



INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification ⁵ : C12N 9/24	A2	(11) International Publication Number: WO 94/24270 (43) International Publication Date: 27 October 1994 (27.10.94)
(21) International Application Number: PCT/CA94/00180 (22) International Filing Date: 7 April 1994 (07.04.94) (30) Priority Data: 08/044,621 8 April 1993 (08.04.93) US (60) Parent Application or Grant (63) Related by Continuation US 08/044,621 (CIP) Filed on 8 April 1993 (08.04.93) (71) Applicant (for all designated States except US): NATIONAL RESEARCH COUNCIL OF CANADA [CA/CA]; Building M-58, Montreal Road, Ottawa, Ontario K1A 0R6 (CA). (72) Inventors; and (75) Inventors/Applicants (for US only): CAMPBELL, Robert, L. [CA/CA]; 660 Brome Crescent, Orleans, Ontario K4A 1W2 (CA). ROSE, David, R. [CA/CA]; 33 Colonel Butler Drive, Markham, Ontario L3P 6B6 (CA). SUNG, Wing, L. [CA/CA]; 2148 Fillmore Crescent, Gloucester, Ontario K1J 6A4 (CA). YAGUCHI, Makoto [CA/CA]; Apartment 2201, 1380 Prince of Wales Drive, Ottawa, Ontario K2C 3N5 (CA). WAKARCHUK, Warren, W. [CA/CA]; 11-	(74) Agent: ERRATT, Judy, A.; Gowling, Strathy & Henderson, 160 Elgin Street, Ottawa, Ontario K1P 1C3 (CA). (81) Designated States: BR, CA, FI, JP, US, European patent (AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE). Published <i>Without international search report and to be republished upon receipt of that report.</i>	
(54) Title: STABLE MUTANTS OF A LOW MOLECULAR MASS XYLANASE		
(57) Abstract		
<p>The stability of the 20,396 dalton <i>Bacillus circulans</i> xylanase was increased by site-directed mutagenesis. Increased stability was conferred by the presence of non-native disulfide bridges, and selected N-terminal mutations. The introduction of these non-native disulfide bridges was accomplished by the examination of the three-dimensional structure of the enzyme, and choosing sites where a favorable geometry for a bridge existed. The N-terminal mutations were constructed on the basis of primary sequence comparison with other family G xylanases. The mutant proteins were examined: for their ability to retain enzymatic activity after heating, as an indication of increased thermostability; for their ability to function at elevated temperatures and for their ability to function at a more basic pH. These more stable variants are useful as an alternative to chemical bleaching of Kraft pulp in a pre-bleaching step (bio-bleaching). The pre-bleaching step involves higher temperature and pH than that normally used for these enzymes, and accordingly these variants can be advantageously used at this step. These stable xylanases are also of use in the food processing industry.</p>		

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**STABLE MUTANTS OF A LOW MOLECULAR
MASS XYLANASE**

5 This application is a continuation-in-part of
U.S. application 08/044,621 filed April 8, 1993.

BACKGROUND AND PRIOR ART

10 The present invention is directed to a modified
xylanase, which shows an improved stability when compared
to the naturally occurring xylanase. Specifically the
present invention is directed to a modified xylanase,
wherein said xylanase has increased thermostability,
increased temperature optimum and/or increased pH optimum,
15 and wherein said xylanase is modified through either the
introduction of at least one non-native disulfide bridge,
the introduction of at least one N-terminal mutation, or
combinations thereof.

20 Current strategies for the production of paper
use a chemical bleaching step, which is essential for the
colour and quality of the paper. Chemical bleaching uses
chlorine or chlorine dioxide and produces substantial
amounts of by-products, which are environmental pollutants.
25 The bleaching process can be enhanced by using an enzymatic
pre-treatment with xylanase (Paice and Jurasek, 1984
Journal of Wood Chemistry and Technology, 4(2):187-198),
which lowers the chlorine charge needed to affect
bleaching, thereby reducing pollutants. In addition there
30 is less bleaching chemical used, which lowers the chemical
costs. New bleaching technology using, oxygen or peroxid s
with xylanase, are also as effective in brightening the
pulp.

35 The step in the process where the enzyme is
applied is after a hot alkali treatment, so that the pulp
is very basic and hot. Both of these conditions are
sub-optimal for xylanase enzymatic activity. Many pulp
mills have the capability to acidify the pulp to a pH which

is closer to the pH optimum for the enzyme and the pulp is adjusted from pH 10-11 to pH 6-8. Due to corrosion risk the pH should preferably be higher than 6.5. A xylanase with a higher pH optimum would be advantageous, especially if the pH-adjustment step could be completely eliminated. Cooling the pulp is too energy intensive (expensive) to be used in the mill setting. Therefore, a xylanase, which is active at a higher temperature would be useful in the bio-bleaching processes. According to Nissen et al. (Xylanases for the Pulp and Paper Industry In: Xylans and Xylanases, Ed. J. Visser et al., 1992, Elsevier Science publishers B.V.) the ideal xylanase for the bleaching process would have a temperature optimum of 70°C and a pH optimum of 9.

Xylanase also has uses in non-pulp applications. Xylanases have been reported to be useful in clarifying juice and wine (Zeikus. J.G., Lee, Y.-E., and Saha, B.C. 1991. ACS Symp. Ser. 460:36-51; Beily, P. 1991. ACS Symp. Ser. 460:408-416; Woodward J. 1984. Top Enzyme Ferment. Biotechnol. 8:9-30), extracting coffee, plant oils and starch (McCleary, B.V. 1986. Int. J. Biol. Macromol. 8:349-354; Beily, P. 1991. ACS Symp. Ser. 460:408-416; Woodward J. 1984. Top Enzyme Ferment. Biotechnol. 8:9-30), for the production of food thickeners (Zeikus. J.G., Lee, Y.-E., and Saha, B.C. 1991. ACS Symp. Ser. 460:36-51), altering texture in bakery products (Maat, J., Roza. M., Verbakel, J., Stam, H., Santos da Silva, M.J., Bosse, M., Egmond, M.R., Hagemans, M.L.D., v.Gorcom, R.F.M., Hessing, J.G.M., v.d.Hodel, C.A.M.J.J., and Rotterdam, C. 1992. In Xylans and xylanases. Visser, J., Beldman, G., Kusters-van Someren, M.A. and Voragen, A.G.J., eds. Elsevier Sci pub., Amsterdam. ISBN 0-444-894-772; McCleary, B.V. 1986. Int. J. Biol. Macromol. 8:349-354), and in the washing of super precision devices and semiconductors (Takayuki, I., Shoji, S. US patent number 5078802, issue date 92-01-07). Several of these application could benefit from a thermostable xylanase, for example, food processing at elevated temperatures.

A thermostable xylanase from *Thermoascus aurantiacus* was produced in US Patent 4,966,850 (Yu et al.) from a particular strain of *T. aurantiacus*, while culturing the strain at high temperature culturing conditions, however this enzyme is not a member of the family G xylanases (Gilkes et al. 1991, Microbiol. Reviews 55(2):303-315), which is the subject of this patent.

Arase et al. (FEBS 316:123-127, 1993) report improvements in thermostability of *Bacillus pumilus* xylanase through random mutagenesis of the gene by chemical mutagens. Their improvements in thermostability are minor in comparison to that of the present invention. The prior art most stable mutant maintained 40% residual activity after a short period of 20 minutes at 57°C. This mutant had a low specific activity, equivalent to 19% of the wild type *B. pumilus* xylanase. It is noted that the temperature optimum and pH optimum of these prior art mutants were not studied.

Site directed mutagenesis has been used to produce more stable proteins. Disulfide (SS) bonds in proteins restrict the degree of freedom for the unfolded state and thereby stabilize the folded state. The first type of protein stabilization performed by genetic manipulation was the introduction of disulfide bonds. One or two amino acids in the protein are replaced with cysteines; a disulfide bond forms *in vivo* or *in vitro*. If the introduced disulfide bond causes no or little tertiary structural change, the cross-links stabilizes the protein. Disulfide bonds have been engineered into T4 lysozyme (T4L) (Perry, L.J. and Wetzel, R. (1984) Science 226, 555-557; Wetzel, R., Perry, L.J. Baase, W.A. and Becktel, W.J. (1988) Proc. Nat. Acad. Sci. USA 85, 401-405), subtilisin (Wells, J.A. and Powers, D.B. (1986) J. Biol. Chem. 261,

6564-6570; Mitchinson, C. and Wells, J.A. (198),
dihydrofolate reductase (DHFR) (Villafranca, J.E., Howell,
E.E., Oatley, S.J., Xuong, N. and Kraut, J. (1987)
Biochemistry 26, 2182-2189), and the Phage λ repressor (Cl)
5 (Sauer, R.T., Hehir, K., Stearman, R.S. et al. (1986)
Biochemistry 25, 5992-5998) with stabilization occurring in
some cases but not others.

For example, in T4L the introduction of SS bonds
10 showed an increase in thermostability of between 6 and 11°C
based on reversible denaturation at pH 2 (Matsumura et al,
1989, Nature 342:291-293). This data does not show how
much activity remains after heating the sample, which in a
functional sense is what is important for an industrial
15 enzyme. The RNASE H SS bond mutant is also stabilized by
11.8°C as measured by reversible thermal denaturation, but
has no enzymatic activity (Kanaya et al, 1991, Journal of
Biological Chemistry 226(10):6038-6044). In DHFR the
artificial SS bond contributes to stability of the protein
20 against chemical denaturation, but does not confer
thermostability (Villafranca et al, 1987, Biochemistry
26:2182-2189). A similar situation occurs with subtilisin,
where 5 different engineered SS bonds do not confer
thermostability (Mitchinson and Wells, 1989, Biochemistry
25 28:4807-4815).

SUMMARY OF INVENTION

According to the present invention there is
30 provided a modified xylanase, wherein said xylanase has
increased stability and wherein said xylanase is modified
through either the introduction of at least one non-native
disulfide bridge, the introduction of at least one N-
terminal mutation, or combinations thereof. The modified
35 xylanases of the present invention exhibit at least one of
the following traits: increased thermostability, increased
temperature optimum or increased pH optimum.

In one embodiment of the present invention, the modified xylanase has been modified by the introduction of an intra-molecular disulfide bridge between a cysteine amino acid, which has been introduced on the last strand of sheet III, and a cysteine amino acid, which has been introduced on the alpha helix.

In a further embodiment of the present invention, the modified xylanase has been modified by the introduction of an inter-molecular disulfide bridge between two xylanase molecules, wherein a cysteine amino acid has been introduced in each of said two molecules.

In a further embodiment of the present invention, the modified xylanase has been modified by the introduction of a mutations at the N-terminus of the xylanase.

In one embodiment of the present invention there is provided a modified family G xylanase essentially having the structure of the *B. circulans* enzyme or mutated to essentially have this structure, wherein said xylanase has increased stability and wherein said xylanase is modified through either the introduction of at least one non-native disulfide bridge, the introduction of at least one N-terminal mutation, or combinations thereof;

wherein the disulfide bridge is an intra-molecular bridge between a cysteine amino acid, which has been introduced on the last strand of beta-sheet III, and a cysteine amino acid, which has been introduced on the alpha helix, or on either side, adjacent to the alpha helix or the disulphide bridge is an inter-molecular bridge between two xylanase molecules, wherein a cysteine amino acid has been introduced in each of said two molecules, on the external region; and

wherein the N-terminal mutation is selected from at least one mutation of the group consisting of the introduction of tyrosine at amino acid position 8,

introduction of phenylalanine at amino acid position 8, introduction of proline at amino acid position 22, and introduction of an N-terminal to C-terminal disulfide bridge, and wherein these N-terminal mutations can be used in combination with other N-terminal mutation introduced at amino acid position 1 to 25 of the N-terminal region, based on the amino acid numbering from *B. circulans* xylanase.

In a further embodiment of the present invention there is provided a modified family G xylanase essentially having the structure of the *B. circulans* enzyme or mutated to essentially have this structure, wherein said xylanase has increased stability and wherein said xylanase is modified through either the introduction of at least one non-native disulfide bridge, the introduction of at least one N-terminal mutation, or combinations thereof; and wherein said modified xylanase is produced from clones selected from the group consisting of TS1, TS2, TS3, TS3a, TS5a, TS6a, TS7a, TS10a, TS14a, TS15a, TS17a, TS19a, TS20a and TS21a.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 shows the multiple sequence alignment among low molecular weight xylanases.

Figure 2 shows a stereodiagram of the overall fold of the three-dimensional crystal structure of the *Bacillus circulans* xylanase. The strands of beta-sheet are represented by arrows and the alpha-helix is represented by a cylinder. The three beta-sheets referred to in the text are indicated by I, II, and III.

Figure 3 shows a stereodiagram of the superimposed three-dimensional crystal structures of the xylanases from *B. circulans* and *T. harzianum*. The structures are drawn such that the positions of the alpha-carbons of each

amino acid are linked by a straight line. The *B. circulans* structure is drawn in a thick line and the *T. harzianum* structure is drawn in a thin line. The *T. harzianum* xylanase has a slightly more open active site due to different intermolecular crystal contacts.

Figure 4 shows a stereodiagram of the superimposed structures of the wild-type and disulfide-containing mutant (TS1) of the *B. circulans* xylanase in the vicinity of the mutation (residues 100 and 148). The wild-type enzyme is drawn in thick lines and the mutant is drawn in thin lines.

Figure 5 shows a stereodiagram of the superimposed structures of the xylanases from *B. circulans* and *T. harzianum* in the vicinity of the disulfide bond shown in Figure 4. The *B. circulans* structure is drawn in a thick line and the *T. harzianum* structure is drawn in a thin line.

Figure 6 shows the native sequence (SEQ ID NO:1) of the *B. subtilis* xylanase gene from plasmid pBSX. The binding sites for the PCR primers and the S100C mutagenic primer are underlined.

Figure 7 shows the semi-synthetic gene sequence (SEQ ID NO:2) for *B. circulans* xylanases. The sites for UDNA mutagenesis to produce TS2 are shown with underlining.

Figure 8 shows the SDS PAGE results of monomer and dimer fraction from TS4a, TS4M and TS4D. Lane 1 is TS4a monomer fraction, reduced; Lane 2 is as in lane 1 but non-reduced; Lane 3 is TS4a dimer fraction, reduced; Lane 4 is as lane 3 but non-reduced; Lane 5 is TS4M monomer fraction, reduced; Lane 6 is as in lane 5 but non-reduced; Lane 7 is TS4D dimer fraction reduced; Lane 8 is as lane 7 but non-reduced; Lane 9 is BCX wild type reduced; Lane 10

is as in lane 9 but non-reduced. For lanes 1-4, approximately 1 μ g of protein was loaded and for the other lanes, approximately 2 μ g was loaded.

5 Figure 9 shows the complete synthetic gene sequence (SEQ ID NO:3) encoding the *B. circulans* xylanase in the plasmid pXYbc.

10 Figure 10 shows the electrophoretic mobility of the disulfide bridge containing mutants of *B. circulans* xylanase. Lane 1 shows the molecular weight standard, lane 2 is the BCX wild-type, reduced, lane 3 is as in lane 2 but non-reduced, lane 4 is the TS1 mutant, reduced, lane 5 is the TS1 mutant, non-reduced, lane 6 is the TS2 mutant, reduced and lane 7 is a TS2 mutant, non-reduced.

15 Figure 11 shows a comparison of the thermostability at 58°C of various mutants of *B. circulans* xylanase. The curve shown for TS4 is for the mixture of both monomer and dimer.

20 Figure 12 shows a comparison of the thermostability at 61°C of various mutants of the *B. circulans* xylanases. The curve shown for TS4 is for the mixture of both monomer and dimer.

25 Figure 13 shows the thermostability of the TS4a (S179C) dimer at 58°C.

30 Figure 14 shows the thermostability at 58°C of *B. circulans* xylanase mutants TS3 and TS4D, which are combinations of mutants shown in Figures 11 and 12.

35 Figure 15 shows the thermostability at 62°C of *B. circulans* xylanase mutants TS3 and TS4D, which are combinations of mutants shown in Figures 11 and 12.

Figure 16 shows the thermostability at 64°C of *B. circulans* xylanase mutants TS3 and TS4D, which are combinations of mutations shown in Figures 11 and 12.

Figure 17 illustrates the effect of temperature on enzyme activity. With the thermostable xylanase mutants shown, an increase of 18°C resulted in between 2.6 and 4 fold increase in activity.

Figure 18 shows the thermostability of xylanase BCX and mutants wherein xylanase from the wild-type or mutant strains were heated at various temperatures for 30 minutes. After cooling to 20°C a residual enzymatic activity of the heated samples were determined via the HBAH assay at 40°C.

Figure 19 shows the molecular structure of residue 6-10 and 16-20 of the N-terminus of the wild-type BCX. CA represents the alpha carbon atom of each residue. CB is the beta-carbon atom of the side-chain. OD1 is the delta oxygen atom in the side-chain of asparagine-8. The number next to CA, CB and OD1 designates the residue to which these atoms belong. The two asterisks are the two buried water molecules. The broken lines represent the hydrogen bonds.

Figure 20 shows the molecular structure of the same region as Figure 19, illustrating the postulated effect of the asparagine to tyrosine mutation at residue-8 (TS5a).

Figure 21 shows the average main-chain B-factors for the xylanase from *B. circulans*. The B-factor is a measure of the spreading out of electron density. It is thus a measure of the mobility of the atoms in a structure. This plot shows the B-factors (or mobility) averaged over all main-chain atoms in each amino acid. Thus the regions near

the amino-terminus and near residue 120 are the most mobile parts of the structure.

5 Figure 22 shows the average main-chain B-factors for the xylanase from *T. harzianum*.

Figure 23 shows the average main-chain B-factors for the disulfide-containing mutant (TS1) of the xylanase from *B. circulans*.

10

Figure 24 shows a Ramachandran plot for the xylanase from *B. circulans*. The two residues (D121 and A165) with main-chain dihedral angles outside of normal limits are labelled. Glycines are shown with circles, while all other amino acids are shown with "plus" signs.

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Figure 25 shows a Ramachandran plot for the xylanase from *T. harzianum*. The three residues (T2, N11 and S181) with main-chain dihedral angles outside of normal limits are labelled. Glycines are shown with circles, while all other amino acids are shown with "plus" signs.

20

Figure 26 shows enzymatic activity of selected xylanase mutants in a thirty minute assay on soluble xylan at temperatures ranging from 40°C to 80°C.

25

Figure 27 shows the enzymatic activity of selected xylanase mutants at a pH ranging from 4 to 10.

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Figure 28 demonstrates the bleaching of pulp at pH 8 by selected xylanase mutants at temperatures ranging from 40°C to 70°C.

DETAILED DESCRIPTION OF THE INVENTION

35

The present invention is related to modified xylanases belonging to the family G xylanases (Henrissat

and Bairoch, Biochem, J. 293: 781-788, 1993 and Gebler et al., J. Biol. Chem. 266: 12559-12561, 1992; incorporated herewith by reference) recently renamed to family 11 (Henrissat and Bairoch, Biochem. J. 293: 7681-788, 1993).
5 The original family G classification was based on the primary sequence comparison and hydrophobic cluster analysis of 4 protein sequences that were in the database at the time the paper, regarding the original classification, was published. Since that time, an
10 additional 16 sequences have been added to this group. In addition to the sequence comparisons, the group definition, also included the stereochemical outcome of the hydrolysis reaction (catalytic mechanism). The grouping by sequence analysis predicts the protein folding will be similar, and
15 the examination of the stereochemistry of the reaction is an indirect measure of how the active site residues are oriented (the prediction is enzymes with similar structure give the same stereochemistry in the reaction products).

20 The complete amino acid sequence of the low molecular weight xylanase has been determined from a number of different bacterial and fungal sources (M. Yaguchi et al., Amino Acid Sequence of the Low-Molecular-Weight Xylanase from *Trichoderma viride*, Xylans and Xylanases, edited
25 by J. Visser et al, 1992, 149-154). The sequence comparison reported in the reference referred above has been extended to show the sequence similarities and differences between the bacteria and fungal family G xylanases as listed below.

BACTERIAL

Bacillus pumilus

Fukusaki, E., Panbangred, W., Shinmyo, A., Okada, H.
FEBS Letters 171:197-201 (1984)

Clostridium acetobutylicum, XYN B

Zappe, H., Jones, W.A., Woods, D.R. Nucleic Acids
Research 18:2179 (1990)

Ruminococcus flavefaciens

Zhang, J., Flint, H.J. EMBL database accession number
Z11127 (1992)

5 *Streptomyces* sp. No. 36a

Nagashima, M., Okumoto, Y., Okanishi, M. Trends
in Actinomycetologia, 91-96 (1989)

Streptomyces lividans, XYN B and XYN C

10 Shareck, F., Roy, C., Yaguchi, M., Morosoli, R.,
Kluepfel, D. Gene, 107:75-82 (1991)

Bacillus circulans

Yang, R.C.A., MacKenzie, C.R., Narang, R.A.
Nucleic Acids Res. 16:7187 (1988)

Bacillus subtilis

15 Paice, M.G., Bourbonnais, R., Desrochers, M.,
Jurasek, L., Yaguchi, M. Arch. Microbiol.
144:201-206 (1986)

FUNGAL

20 *Trichoderma reesei*, XYN I and XYN II

Torronene, A., Mach, R.L., Messner, R.,
Gonzalez, R., Kalkkinen, N., Harkki, A.,
Kubicek, C.P. Bio/Technology 10:1461-1465 (1992)

Trichoderma viride, 20KD

25 Yaguchi, M., Roy, C., Ujlie, M., Watson, D.C.,
Wakarchuk, W. Xylans and Xylanases, ed. by J.
Visser et al., Elsevier, pp. 149-154 (1992)

Trichoderma harzianum, 20KD

30 Yaguchi, M., Roy, C., Watson, D.C., Rollin, F.,
Tan, L.U.L., Senior, D.J., Saddler, J.N. Xylans
and Xylanases, ed. by J. Visser et al.,
Elsevier, pp. 435-438 (1992)

Schizophyllum commune, Xylanase A

35 Oku, T., Roy, C., Watson, D.C., Wakarchuk, W.,
Yaguchi, M., Jurasek, L., Paice, M.G.
(unpublished)

Aspergillus niger var. *awamori*

Maat, J., Roza, M., Verbakel, J., Stam, H.,
Santos da Silva, M.J., Egmond, M.R., Hagemans,
M.L.D., Gorcom, R.F.M.v., Hessing, J.G.M.,
Hondel, C.A.M.J.J.v.d., Rotterdam, C.v. Xylans
and Xylanases, ed. by J. Visser et al.,
Elsevier, pp. 349-360 (1992)

Aspergillus tubigensis, XYL A

de Graaff, L.H., van den Broeck, H.C., van
Ooijan, A.J.J., Visser, J. Xylans and Xylanases,
ed. by J. Visser et al., Elsevier, pp. 235-246
(1992)

Figure 1 shows a multiple sequence alignment
among low molecular mass xylanases obtained with GeneWorks
version 2.2.1 (IntelliGenetics, Inc., Mountain View, CA),
which has been manually edited to conform to the structural
homology between the xylanases from *B. circulans* and *T.*
harzianum. The extended N-terminal sequence of the *C.*
acetobutylicum xylanase B (residues 1-31) and the C-terminal
sequences of *S. lividans*, xylanase B (residues 216-293) are
not shown.

Table 1 shows the amino acid sequence identity
(percentage) between different groups of family G
xylanases, when compared to *B. pumilus*, *B. circulans*, *T.*
harzianum and *Schizo. commune* as references. Due to the
sequence homology among related xylanases, one could expect
that mutations for the introduction of SS bonds or for the
introduction of mutations at the N-terminal end of the
xylanase, as demonstrated in the examples below for *B.*
circulans xylanase, can be extended to other xylanases from
bacterial or fungal sources to produce similar effects.

Table 1

Amino Acid Sequence Identity (%) between the Family G Xylanases

	<i>Bacillus pumilus</i>	<i>Bacillus circulans</i>	<i>Trichoderma harzianum</i>	<i>Schizo. commune</i>
<u>Bacterial</u>				
<i>B. pumilus</i>	-	43	46	40
<i>C. acetobutylicum</i>	71	42	42	41
<i>R. flavefaciens</i>	46	36	41	39
<i>Strept. sp. 36a</i>	49	57	50	47
<i>S. lividans, B</i>	50	56	51	47
<i>S. lividans, C</i>	49	60	52	51
<i>B. circulans</i>	43	-	51	50
<i>B. subtilis</i>	43	99	51	50
<u>Fungal</u>				
<i>T. reesei, II</i>	47	51	95	53
<i>T. viride</i>	48	50	94	53
<i>T. harzianum</i>	46	51	-	54
<i>S. commune</i>	40	50	54	-
<i>A. niger awamori</i>	34	42	41	38
<i>A. tubigenensis, A</i>	34	43	41	37
<i>T. reesei, I</i>	37	46	50	38

The xylanase from *B. circulans* is functionally identical to that from *B. subtilis*, which will be seen later in



the Examples. These proteins differ at only one residue and are among the shortest xylanases, with their N-terminus lacking at least 10 amino acid residues compared to other xylanases.

5

The three-dimensional crystal structure of the *B. circulans* xylanase is represented in Figure 2. This ribbon representation shows that the structure is composed of three beta-sheets and one alpha-helix. The first two beta-sheets are roughly parallel, while sheet III is at about a 90° angle to sheet II. Sheets I and II are each composed of five strands, while sheet III contains 6 strands. The alpha-helix lies across the back of sheet III and the last two strands of sheet III fold over one edge of the alpha-helix. The active site lies in the cleft between sheets II and III. The x-ray co-ordinates of the structure is given below.

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ATOM	1	CB	ALA	1	32.404	42.580	22.419
1.00	19.66						
ATOM	2	C	ALA	1	34.898	42.615	22.344
1.00	20.06						
ATOM	3	O	ALA	1	35.540	41.613	22.023
1.00	20.55						
ATOM	6	N	ALA	1	33.610	42.325	20.269
1.00	18.68						
ATOM	8	CA	ALA	1	33.627	42.997	21.599
1.00	19.67						
ATOM	9	N	SER	2	35.283	43.440	23.308
1.00	20.15						
ATOM	11	CA	SER	2	36.455	43.158	24.114
1.00	20.60						
ATOM	12	CB	SER	2	37.000	44.436	24.753
1.00	22.52						
ATOM	13	OG	SER	2	37.614	45.262	23.783
1.00	25.52						
ATOM	15	C	SER	2	36.062	42.184	25.210
1.00	20.08						
ATOM	16	O	SER	2	34.967	42.270	25.786
1.00	19.93						
ATOM	17	N	THR	3	36.930	41.215	25.440
1.00	18.98						
ATOM	19	CA	THR	3	36.715	40.235	26.475
1.00	18.01						
ATOM	20	CB	THR	3	37.469	38.943	26.145
1.00	18.17						
ATOM	21	OG1	THR	3	38.849	39.247	25.891
1.00	17.58						

	ATOM	23	CG2	THR	3	36.860	38.273	24.920
	1.00	17.34						
	ATOM	24	C	THR	3	37.306	40.884	27.713
	1.00	17.67						
5	ATOM	25	O	THR	3	38.232	41.694	27.610
	1.00	18.99						
	ATOM	26	N	ASP	4	36.739	40.601	28.874
	1.00	16.43						
	ATOM	28	CA	ASP	4	37.252	41.190	30.104
10	1.00	16.02						
	ATOM	29	CB	ASP	4	36.284	42.252	30.644
	1.00	16.80						
	ATOM	30	CG	ASP	4	34.886	41.706	30.907
	1.00	19.10						
15	ATOM	31	OD1	ASP	4	34.741	40.512	31.221
	1.00	17.29						
	ATOM	32	OD2	ASP	4	33.923	42.495	30.810
	1.00	21.94						
	ATOM	33	C	ASP	4	37.506	40.143	31.161
20	1.00	15.35						
	ATOM	34	O	ASP	4	37.721	40.470	32.325
	1.00	16.73						
	ATOM	35	N	TYR	5	37.455	38.875	30.769
	1.00	13.80						
25	ATOM	37	CA	TYR	5	37.665	37.812	31.722
	1.00	12.53						
	ATOM	38	CB	TYR	5	36.318	37.186	32.119
	1.00	12.90						
	ATOM	39	CG	TYR	5	36.430	36.223	33.270
30	1.00	14.19						
	ATOM	40	CD1	TYR	5	36.583	36.679	34.577
	1.00	15.98						
	ATOM	41	CE1	TYR	5	36.748	35.786	35.632
	1.00	17.93						
35	ATOM	42	CD2	TYR	5	36.438	34.855	33.052
	1.00	14.54						
	ATOM	43	CE2	TYR	5	36.603	33.966	34.092
	1.00	16.97						
	ATOM	44	CZ	TYR	5	36.762	34.431	35.379
40	1.00	17.23						
	ATOM	45	OH	TYR	5	36.972	33.528	36.401
	1.00	21.34						
	ATOM	47	C	TYR	5	38.610	36.754	31.175
	1.00	12.09						
45	ATOM	48	O	TYR	5	38.539	36.387	29.996
	1.00	11.58						
	ATOM	49	N	TRP	6	39.523	36.309	32.027
	1.00	11.81						
	ATOM	51	CA	TRP	6	40.498	35.270	31.691
50	1.00	12.62						
	ATOM	52	CB	TRP	6	41.922	35.830	31.788
	1.00	12.94						
	ATOM	53	CG	TRP	6	43.050	34.813	31.806
	1.00	12.88						
55	ATOM	54	CD2	TRP	6	43.420	33.895	30.761
	1.00	12.72						



	ATOM	55	CE2	TRP	6	44.595	33.232	31.184
	1.00	13.51						
	ATOM	56	CE3	TRP	6	42.879	33.570	29.515
	1.00	13.01						
5	ATOM	57	CD1	TRP	6	43.982	34.661	32.791
	1.00	13.74						
	ATOM	58	NE1	TRP	6	44.912	33.718	32.425
	1.00	14.48						
10	ATOM	60	CZ2	TRP	6	45.236	32.271	30.404
	1.00	13.34						
	ATOM	61	CZ3	TRP	6	43.518	32.607	28.740
	1.00	13.00						
	ATOM	62	CH2	TRP	6	44.681	31.974	29.187
	1.00	12.55						
15	ATOM	63	C	TRP	6	40.292	34.122	32.670
	1.00	12.15						
	ATOM	64	O	TRP	6	40.399	34.289	33.890
	1.00	12.46						
20	ATOM	65	N	GLN	7	39.918	32.974	32.118
	1.00	12.04						
	ATOM	67	CA	GLN	7	39.656	31.763	32.877
	1.00	12.76						
	ATOM	68	CB	GLN	7	38.380	31.105	32.332
	1.00	13.89						
25	ATOM	69	CG	GLN	7	38.105	29.698	32.821
	1.00	16.24						
	ATOM	70	CD	GLN	7	37.879	29.624	34.314
	1.00	17.99						
30	ATOM	71	OE1	GLN	7	37.712	30.644	34.993
	1.00	19.93						
	ATOM	72	NE2	GLN	7	37.867	28.411	34.838
	1.00	20.16						
	ATOM	75	C	GLN	7	40.843	30.818	32.726
	1.00	12.58						
35	ATOM	76	O	GLN	7	41.211	30.455	31.612
	1.00	11.22						
	ATOM	77	N	ASN	8	41.471	30.451	33.837
	1.00	12.68						
40	ATOM	79	CA	ASN	8	42.615	29.550	33.784
	1.00	13.88						
	ATOM	80	CB	ASN	8	43.924	30.351	33.687
	1.00	15.02						
	ATOM	81	CG	ASN	8	45.166	29.462	33.674
	1.00	16.98						
45	ATOM	82	OD1	ASN	8	46.279	29.935	33.916
	1.00	20.52						
	ATOM	83	ND2	ASN	8	44.990	28.192	33.377
	1.00	17.00						
50	ATOM	86	C	ASN	8	42.604	28.712	35.045
	1.00	14.62						
	ATOM	87	O	ASN	8	43.215	29.075	36.057
	1.00	15.63						
	ATOM	88	N	TRP	9	41.894	27.594	34.978
	1.00	14.02						
55	ATOM	90	CA	TRP	9	41.766	26.703	36.113
	1.00	14.57						

	ATOM	91	CB	TRP	9	40.300	26.630	36.562
	1.00	16.93						
	ATOM	92	CG	TRP	9	40.058	25.646	37.680
	1.00	19.06						
5	ATOM	93	CD2	TRP	9	39.703	24.260	37.548
	1.00	19.90						
	ATOM	94	CE2	TRP	9	39.600	23.728	38.851
	1.00	20.63						
	ATOM	95	CE3	TRP	9	39.462	23.420	36.455
10	1.00	20.29						
	ATOM	96	CD1	TRP	9	40.151	25.888	39.025
	1.00	20.86						
	ATOM	97	NE1	TRP	9	39.879	24.740	39.731
	1.00	21.73						
15	ATOM	99	CZ2	TRP	9	39.268	22.397	39.090
	1.00	20.83						
	ATOM	100	CZ3	TRP	9	39.133	22.100	36.694
	1.00	20.61						
	ATOM	101	CH2	TRP	9	39.038	21.600	38.003
20	1.00	20.23						
	ATOM	102	C	TRP	9	42.256	25.300	35.799
	1.00	14.32						
	ATOM	103	O	TRP	9	41.974	24.757	34.732
	1.00	13.18						
25	ATOM	104	N	THR	10	42.978	24.714	36.745
	1.00	13.98						
	ATOM	106	CA	THR	10	43.461	23.352	36.609
	1.00	14.97						
	ATOM	107	CB	THR	10	44.929	23.291	36.133
30	1.00	15.94						
	ATOM	108	OG1	THR	10	45.385	21.934	36.177
	1.00	17.17						
	ATOM	110	CG2	THR	10	45.831	24.146	37.021
	1.00	17.26						
35	ATOM	111	C	THR	10	43.362	22.696	37.976
	1.00	15.04						
	ATOM	112	O	THR	10	43.419	23.378	39.000
	1.00	15.78						
	ATOM	113	N	ASP	11	43.145	21.387	38.000
40	1.00	15.06						
	ATOM	115	CA	ASP	11	43.101	20.686	39.277
	1.00	16.34						
	ATOM	116	CB	ASP	11	42.200	19.448	39.228
	1.00	16.43						
45	ATOM	117	CG	ASP	11	42.629	18.417	38.186
	1.00	16.04						
	ATOM	118	OD1	ASP	11	43.738	18.498	37.612
	1.00	16.20						
	ATOM	119	OD2	ASP	11	41.819	17.506	37.945
50	1.00	17.65						
	ATOM	120	C	ASP	11	44.529	20.336	39.724
	1.00	17.44						
	ATOM	121	O	ASP	11	44.723	19.661	40.731
	1.00	18.70						
55	ATOM	122	N	GLY	12	45.517	20.780	38.946
	1.00	17.45						



	ATOM	124	CA	GLY	12	46.913	20.547	39.287
	1.00	17.91						
	ATOM	125	C	GLY	12	47.616	19.394	38.593
	1.00	17.48						
5	ATOM	126	O	GLY	12	48.841	19.251	38.699
	1.00	18.34						
	ATOM	127	N	GLY	13	46.862	18.568	37.881
	1.00	16.38						
10	ATOM	129	CA	GLY	13	47.466	17.443	37.202
	1.00	15.25						
	ATOM	130	C	GLY	13	48.141	17.771	35.887
	1.00	15.48						
	ATOM	131	O	GLY	13	47.608	18.530	35.070
	1.00	15.97						
15	ATOM	132	N	GLY	14	49.319	17.187	35.687
	1.00	14.01						
	ATOM	134	CA	GLY	14	50.062	17.366	34.456
	1.00	13.22						
20	ATOM	135	C	GLY	14	50.476	18.783	34.128
	1.00	13.48						
	ATOM	136	O	GLY	14	50.581	19.642	35.009
	1.00	15.09						
	ATOM	137	N	ILE	15	50.707	19.026	32.845
	1.00	12.64						
25	ATOM	139	CA	ILE	15	51.145	20.327	32.387
	1.00	13.51						
	ATOM	140	CB	ILE	15	52.415	20.196	31.469
	1.00	16.01						
30	ATOM	141	CG2	ILE	15	52.750	21.523	30.777
	1.00	16.26						
	ATOM	142	CG1	ILE	15	53.615	19.720	32.291
	1.00	17.95						
	ATOM	143	CD1	ILE	15	53.595	18.263	32.618
	1.00	22.36						
35	ATOM	144	C	ILE	15	50.054	21.032	31.604
	1.00	11.40						
	ATOM	145	O	ILE	15	49.447	20.438	30.715
	1.00	11.13						
40	ATOM	146	N	VAL	16	49.780	22.276	31.984
	1.00	11.65						
	ATOM	148	CA	VAL	16	48.811	23.124	31.291
	1.00	11.43						
	ATOM	149	CB	VAL	16	47.501	23.332	32.103
	1.00	12.58						
45	ATOM	150	CG1	VAL	16	46.539	24.263	31.332
	1.00	13.92						
	ATOM	151	CG2	VAL	16	46.833	21.989	32.368
	1.00	12.26						
50	ATOM	152	C	VAL	16	49.515	24.464	31.084
	1.00	12.47						
	ATOM	153	O	VAL	16	49.699	25.225	32.028
	1.00	14.76						
	ATOM	154	N	ASN	17	50.019	24.692	29.879
	1.00	11.15						
55	ATOM	156	CA	ASN	17	50.698	25.945	29.566
	1.00	11.18						

	ATOM	157	CB	ASN	17	51.909	25.681	28.660
	1.00	12.52						
	ATOM	158	CG	ASN	17	52.558	26.962	28.153
	1.00	13.85						
5	ATOM	159	OD1	ASN	17	52.808	27.102	26.954
	1.00	17.56						
	ATOM	160	ND2	ASN	17	52.840	27.888	29.049
	1.00	14.11						
	ATOM	163	C	ASN	17	49.674	26.840	28.871
10	1.00	11.71						
	ATOM	164	O	ASN	17	49.446	26.720	27.663
	1.00	12.32						
	ATOM	165	N	ALA	18	49.038	27.706	29.654
	1.00	11.86						
15	ATOM	167	CA	ALA	18	48.014	28.616	29.143
	1.00	12.70						
	ATOM	168	CB	ALA	18	46.831	28.682	30.114
	1.00	12.87						
	ATOM	169	C	ALA	18	48.601	29.999	28.941
20	1.00	13.74						
	ATOM	170	O	ALA	18	49.201	30.566	29.856
	1.00	14.88						
	ATOM	171	N	VAL	19	48.415	30.551	27.751
	1.00	13.07						
25	ATOM	173	CA	VAL	19	48.925	31.871	27.429
	1.00	13.91						
	ATOM	174	CB	VAL	19	49.800	31.839	26.167
	1.00	14.35						
	ATOM	175	CG1	VAL	19	50.307	33.240	25.850
30	1.00	15.62						
	ATOM	176	CG2	VAL	19	50.964	30.862	26.357
	1.00	16.11						
	ATOM	177	C	VAL	19	47.790	32.865	27.207
	1.00	13.48						
35	ATOM	178	O	VAL	19	46.901	32.643	26.384
	1.00	12.27						
	ATOM	179	N	ASN	20	47.827	33.949	27.965
	1.00	13.30						
	ATOM	181	CA	ASN	20	46.843	35.016	27.877
40	1.00	14.23						
	ATOM	182	CB	ASN	20	46.747	35.697	29.247
	1.00	14.63						
	ATOM	183	CG	ASN	20	45.715	36.812	29.294
	1.00	16.43						
45	ATOM	184	OD1	ASN	20	45.222	37.266	28.275
	1.00	16.62						
	ATOM	185	ND2	ASN	20	45.390	37.255	30.501
	1.00	18.39						
	ATOM	188	C	ASN	20	47.395	35.971	26.813
50	1.00	15.00						
	ATOM	189	O	ASN	20	48.271	36.786	27.107
	1.00	15.64						
	ATOM	190	N	GLY	21	46.941	35.814	25.571
	1.00	13.96						
55	ATOM	192	CA	GLY	21	47.432	36.642	24.481
	1.00	14.20						



	ATOM	193	C	GLY	21	46.799	38.013	24.356
	1.00	14.39						
	ATOM	194	O	GLY	21	46.039	38.438	25.223
	1.00	14.16						
5	ATOM	195	N	SER	22	47.115	38.719	23.271
	1.00	14.12						
	ATOM	197	CA	SER	22	46.560	40.051	23.061
	1.00	15.16						
10	ATOM	198	CB	SER	22	47.327	40.815	21.970
	1.00	17.14						
	ATOM	199	OG	SER	22	47.248	40.141	20.732
	1.00	22.61						
	ATOM	201	C	SER	22	45.083	39.974	22.692
	1.00	14.03						
15	ATOM	202	O	SER	22	44.634	39.007	22.060
	1.00	13.62						
	ATOM	203	N	GLY	23	44.339	41.001	23.090
	1.00	13.56						
	ATOM	205	CA	GLY	23	42.925	41.053	22.791
20	1.00	12.00						
	ATOM	206	C	GLY	23	42.198	39.826	23.305
	1.00	11.46						
	ATOM	207	O	GLY	23	42.338	39.444	24.461
	1.00	11.59						
25	ATOM	208	N	GLY	24	41.429	39.199	22.425
	1.00	10.58						
	ATOM	210	CA	GLY	24	40.682	38.019	22.812
	1.00	9.97						
	ATOM	211	C	GLY	24	41.371	36.717	22.458
30	1.00	10.21						
	ATOM	212	O	GLY	24	40.736	35.663	22.451
	1.00	9.66						
	ATOM	213	N	ASN	25	42.675	36.766	22.203
	1.00	9.53						
35	ATOM	215	CA	ASN	25	43.413	35.559	21.846
	1.00	8.48						
	ATOM	216	CB	ASN	25	44.532	35.893	20.833
	1.00	9.35						
	ATOM	217	CG	ASN	25	45.356	34.680	20.455
40	1.00	10.64						
	ATOM	218	OD1	ASN	25	46.499	34.512	20.908
	1.00	12.41						
	ATOM	219	ND2	ASN	25	44.790	33.823	19.620
	1.00	10.48						
45	ATOM	222	C	ASN	25	44.048	34.839	23.033
	1.00	8.98						
	ATOM	223	O	ASN	25	44.522	35.469	23.976
	1.00	9.94						
	ATOM	224	N	TYR	26	44.030	33.513	22.991
50	1.00	8.04						
	ATOM	226	CA	TYR	26	44.696	32.715	24.016
	1.00	8.17						
	ATOM	227	CB	TYR	26	43.802	32.457	25.243
	1.00	8.24						
55	ATOM	228	CG	TYR	26	42.670	31.472	25.023
	1.00	8.00						

	ATOM	229	CD1	TYR	26	41.414	31.913	24.619
	1.00	9.02						
	ATOM	230	CE1	TYR	26	40.379	31.030	24.437
	1.00	8.79						
5	ATOM	231	CD2	TYR	26	42.851	30.108	25.240
	1.00	8.18						
	ATOM	232	CE2	TYR	26	41.815	29.210	25.057
	1.00	9.20						
	ATOM	233	CZ	TYR	26	40.577	29.682	24.652
10	1.00	8.70						
	ATOM	234	OH	TYR	26	39.534	28.794	24.438
	1.00	9.05						
	ATOM	236	C	TYR	26	45.122	31.403	23.385
	1.00	9.00						
15	ATOM	237	O	TYR	26	44.634	31.027	22.305
	1.00	8.46						
	ATOM	238	N	SER	27	46.087	30.735	24.007
	1.00	9.44						
	ATOM	240	CA	SER	27	46.528	29.440	23.516
20	1.00	9.71						
	ATOM	241	CB	SER	27	47.759	29.566	22.604
	1.00	11.14						
	ATOM	242	OG	SER	27	48.833	30.187	23.275
	1.00	14.81						
25	ATOM	244	C	SER	27	46.809	28.543	24.701
	1.00	9.94						
	ATOM	245	O	SER	27	46.985	29.013	25.825
	1.00	10.37						
	ATOM	246	N	VAL	28	46.728	27.245	24.471
30	1.00	9.16						
	ATOM	248	CA	VAL	28	46.994	26.271	25.520
	1.00	10.37						
	ATOM	249	CB	VAL	28	45.692	25.668	26.146
	1.00	11.40						
35	ATOM	250	CG1	VAL	28	46.023	24.931	27.454
	1.00	12.25						
	ATOM	251	CG2	VAL	28	44.641	26.726	26.377
	1.00	13.82						
	ATOM	252	C	VAL	28	47.724	25.086	24.929
40	1.00	10.81						
	ATOM	253	O	VAL	28	47.402	24.644	23.820
	1.00	11.31						
	ATOM	254	N	ASN	29	48.745	24.619	25.642
	1.00	10.65						
45	ATOM	256	CA	ASN	29	49.484	23.412	25.275
	1.00	12.10						
	ATOM	257	CB	ASN	29	50.977	23.683	25.060
	1.00	15.51						
	ATOM	258	CG	ASN	29	51.225	24.717	24.004
50	1.00	19.33						
	ATOM	259	OD1	ASN	29	50.951	24.496	22.820
	1.00	22.89						
	ATOM	260	ND2	ASN	29	51.718	25.868	24.420
	1.00	21.25						
55	ATOM	263	C	ASN	29	49.322	22.597	26.539
	1.00	10.79						



	ATOM	264	O	ASN	29	49.648	23.078	27.620
	1.00	12.04						
	ATOM	265	N	TRP	30	48.787	21.392	26.430
	1.00	9.27						
5	ATOM	267	CA	TRP	30	48.589	20.575	27.619
	1.00	7.76						
	ATOM	268	CB	TRP	30	47.115	20.598	28.066
	1.00	7.93						
10	ATOM	269	CG	TRP	30	46.123	19.856	27.209
	1.00	7.36						
	ATOM	270	CD2	TRP	30	45.383	20.374	26.090
	1.00	7.38						
	ATOM	271	CE2	TRP	30	44.448	19.387	25.719
	1.00	6.82						
15	ATOM	272	CE3	TRP	30	45.411	21.580	25.379
	1.00	8.62						
	ATOM	273	CD1	TRP	30	45.632	18.610	27.444
	1.00	6.99						
20	ATOM	274	NE1	TRP	30	44.618	18.321	26.562
	1.00	7.92						
	ATOM	276	CZ2	TRP	30	43.542	19.568	24.657
	1.00	9.07						
	ATOM	277	CZ3	TRP	30	44.510	21.759	24.330
	1.00	7.97						
25	ATOM	278	CH2	TRP	30	43.592	20.757	23.982
	1.00	7.80						
	ATOM	279	C	TRP	30	49.112	19.166	27.431
	1.00	7.73						
30	ATOM	280	O	TRP	30	49.151	18.641	26.305
	1.00	8.50						
	ATOM	281	N	SER	31	49.532	18.553	28.530
	1.00	8.50						
	ATOM	283	CA	SER	31	50.095	17.218	28.466
	1.00	9.39						
35	ATOM	284	CB	SER	31	51.615	17.333	28.268
	1.00	11.08						
	ATOM	285	OG	SER	31	52.197	16.069	28.032
	1.00	16.62						
40	ATOM	287	C	SER	31	49.799	16.425	29.735
	1.00	8.65						
	ATOM	288	O	SER	31	50.040	16.912	30.846
	1.00	9.67						
	ATOM	289	N	ASN	32	49.246	15.224	29.556
	1.00	9.23						
45	ATOM	291	CA	ASN	32	48.934	14.290	30.648
	1.00	9.24						
	ATOM	292	CB	ASN	32	50.215	13.581	31.076
	1.00	11.30						
50	ATOM	293	CG	ASN	32	50.856	12.828	29.931
	1.00	13.54						
	ATOM	294	OD1	ASN	32	50.311	11.835	29.448
	1.00	15.18						
	ATOM	295	ND2	ASN	32	52.010	13.300	29.487
	1.00	14.28						
55	ATOM	298	C	ASN	32	48.306	14.979	31.844
	1.00	9.76						

	ATOM	299	O	ASN	32	48.778	14.870	32.975
	1.00	10.47						
	ATOM	300	N	THR	33	47.187	15.634	31.589
	1.00	9.79						
5	ATOM	302	CA	THR	33	46.510	16.413	32.613
	1.00	9.75						
	ATOM	303	CB	THR	33	45.734	17.580	31.943
	1.00	10.19						
10	ATOM	304	OG1	THR	33	44.705	17.033	31.099
	1.00	10.42						
	ATOM	306	CG2	THR	33	46.668	18.456	31.117
	1.00	10.04						
	ATOM	307	C	THR	33	45.471	15.679	33.450
	1.00	9.02						
15	ATOM	308	O	THR	33	45.203	14.490	33.268
	1.00	9.65						
	ATOM	309	N	GLY	34	44.930	16.436	34.397
	1.00	9.55						
20	ATOM	311	CA	GLY	34	43.804	15.992	35.187
	1.00	9.51						
	ATOM	312	C	GLY	34	42.716	16.743	34.416
	1.00	9.70						
	ATOM	313	O	GLY	34	42.654	16.646	33.183
	1.00	9.59						
25	ATOM	314	N	ASN	35	41.924	17.563	35.098
	1.00	9.04						
	ATOM	316	CA	ASN	35	40.873	18.355	34.450
	1.00	9.43						
30	ATOM	317	CB	ASN	35	39.534	18.158	35.187
	1.00	10.15						
	ATOM	318	CG	ASN	35	38.361	18.897	34.531
	1.00	12.88						
	ATOM	319	OD1	ASN	35	37.501	19.427	35.232
	1.00	15.72						
35	ATOM	320	ND2	ASN	35	38.301	18.905	33.204
	1.00	13.33						
	ATOM	323	C	ASN	35	41.290	19.823	34.496
	1.00	9.12						
40	ATOM	324	O	ASN	35	41.876	20.282	35.476
	1.00	10.17						
	ATOM	325	N	PHE	36	41.061	20.545	33.406
	1.00	8.58						
	ATOM	327	CA	PHE	36	41.396	21.966	33.357
	1.00	7.71						
45	ATOM	328	CB	PHE	36	42.832	22.193	32.856
	1.00	9.56						
	ATOM	329	CG	PHE	36	43.018	21.898	31.389
	1.00	9.71						
	ATOM	330	CD1	PHE	36	42.835	22.898	30.434
50	1.00	9.80						
	ATOM	331	CD2	PHE	36	43.322	20.618	30.959
	1.00	9.86						
	ATOM	332	CE1	PHE	36	42.947	22.618	29.082
	1.00	10.32						
55	ATOM	333	CE2	PHE	36	43.437	20.335	29.600
	1.00	11.13						

	ATOM	334	CZ	PHE	36	43.247	21.337	28.667
	1.00	10.13						
	ATOM	335	C	PHE	36	40.433	22.652	32.407
	1.00	7.24						
5	ATOM	336	O	PHE	36	39.856	22.003	31.528
	1.00	8.20						
	ATOM	337	N	VAL	37	40.269	23.956	32.589
	1.00	7.92						
10	ATOM	339	CA	VAL	37	39.405	24.776	31.739
	1.00	8.27						
	ATOM	340	CB	VAL	37	38.007	25.044	32.359
	1.00	8.91						
	ATOM	341	CG1	VAL	37	37.165	25.888	31.382
	1.00	10.27						
15	ATOM	342	CG2	VAL	37	37.300	23.735	32.679
	1.00	10.16						
	ATOM	343	C	VAL	37	40.109	26.109	31.568
	1.00	8.48						
	ATOM	344	O	VAL	37	40.426	26.792	32.556
20	1.00	9.26						
	ATOM	345	N	VAL	38	40.356	26.474	30.315
	1.00	7.80						
	ATOM	347	CA	VAL	38	41.027	27.727	29.988
	1.00	8.41						
25	ATOM	348	CB	VAL	38	42.445	27.453	29.421
	1.00	9.47						
	ATOM	349	CG1	VAL	38	43.098	28.748	28.947
	1.00	11.38						
30	ATOM	350	CG2	VAL	38	43.305	26.766	30.470
	1.00	10.26						
	ATOM	351	C	VAL	38	40.217	28.451	28.921
	1.00	8.22						
	ATOM	352	O	VAL	38	39.717	27.825	28.002
	1.00	9.27						
35	ATOM	353	N	GLY	39	40.091	29.763	29.029
	1.00	8.83						
	ATOM	355	CA	GLY	39	39.344	30.479	28.013
	1.00	8.67						
	ATOM	356	C	GLY	39	39.214	31.960	28.280
40	1.00	9.03						
	ATOM	357	O	GLY	39	39.600	32.449	29.348
	1.00	10.05						
	ATOM	358	N	LYS	40	38.703	32.676	27.287
	1.00	8.28						
45	ATOM	360	CA	LYS	40	38.493	34.109	27.411
	1.00	7.76						
	ATOM	361	CB	LYS	40	39.372	34.892	26.432
	1.00	8.70						
50	ATOM	362	CG	LYS	40	40.787	35.076	26.926
	1.00	10.94						
	ATOM	363	CD	LYS	40	41.525	36.071	26.066
	1.00	10.75						
	ATOM	364	CE	LYS	40	42.861	36.392	26.700
	1.00	11.72						
55	ATOM	365	NZ	LYS	40	43.653	37.312	25.843
	1.00	10.91						

	ATOM	369	C	LYS	40	37.033	34.432	27.172
	1.00	7.68						
	ATOM	370	O	LYS	40	36.346	33.740	26.418
	1.00	8.01						
5	ATOM	371	N	GLY	41	36.567	35.485	27.824
	1.00	7.96						
	ATOM	373	CA	GLY	41	35.189	35.866	27.666
	1.00	8.17						
10	ATOM	374	C	GLY	41	34.807	37.051	28.510
	1.00	8.18						
	ATOM	375	O	GLY	41	35.547	38.042	28.593
	1.00	8.33						
	ATOM	376	N	TRP	42	33.665	36.916	29.174
	1.00	8.49						
15	ATOM	378	CA	TRP	42	33.093	37.988	29.977
	1.00	9.41						
	ATOM	379	CB	TRP	42	31.790	38.455	29.304
	1.00	10.19						
	ATOM	380	CG	TRP	42	32.066	38.913	27.902
20	1.00	10.97						
	ATOM	381	CD2	TRP	42	32.159	38.091	26.725
	1.00	11.39						
	ATOM	382	CE2	TRP	42	32.562	38.926	25.667
	1.00	12.60						
25	ATOM	383	CE3	TRP	42	31.948	36.730	26.469
	1.00	11.60						
	ATOM	384	CD1	TRP	42	32.396	40.174	27.512
	1.00	12.41						
	ATOM	385	NE1	TRP	42	32.702	40.191	26.176
30	1.00	13.46						
	ATOM	387	CZ2	TRP	42	32.761	38.447	24.369
	1.00	12.42						
	ATOM	388	CZ3	TRP	42	32.147	36.254	25.178
	1.00	12.72						
35	ATOM	389	CH2	TRP	42	32.550	37.111	24.147
	1.00	12.03						
	ATOM	390	C	TRP	42	32.851	37.625	31.433
	1.00	9.47						
	ATOM	391	O	TRP	42	32.485	36.498	31.755
40	1.00	9.69						
	ATOM	392	N	THR	43	33.084	38.597	32.309
	1.00	10.28						
	ATOM	394	CA	THR	43	32.924	38.423	33.744
	1.00	11.31						
45	ATOM	395	CB	THR	43	33.385	39.688	34.487
	1.00	13.67						
	ATOM	396	OG1	THR	43	34.716	40.025	34.065
	1.00	16.25						
	ATOM	398	CG2	THR	43	33.393	39.450	35.988
50	1.00	15.27						
	ATOM	399	C	THR	43	31.477	38.108	34.115
	1.00	11.22						
	ATOM	400	O	THR	43	31.219	37.325	35.032
	1.00	11.38						
55	ATOM	401	N	THR	44	30.541	38.720	33.407
	1.00	11.08						

	ATOM	403	CA	THR	44	29.132	38.479	33.658
	1.00	11.81						
	ATOM	404	CB	THR	44	28.429	39.746	34.170
	1.00	13.88						
5	ATOM	405	OG1	THR	44	29.088	40.195	35.361
	1.00	16.33						
	ATOM	407	CG2	THR	44	26.973	39.451	34.497
	1.00	15.15						
10	ATOM	408	C	THR	44	28.474	37.989	32.377
	1.00	10.65						
	ATOM	409	O	THR	44	28.435	38.692	31.364
	1.00	11.08						
	ATOM	410	N	GLY	45	28.034	36.742	32.416
	1.00	8.94						
15	ATOM	412	CA	GLY	45	27.381	36.161	31.267
	1.00	9.08						
	ATOM	413	C	GLY	45	26.024	36.785	31.013
	1.00	8.92						
20	ATOM	414	O	GLY	45	25.426	37.413	31.888
	1.00	10.17						
	ATOM	415	N	SER	46	25.528	36.587	29.803
	1.00	9.11						
	ATOM	417	CA	SER	46	24.233	37.110	29.405
	1.00	9.90						
25	ATOM	418	CB	SER	46	24.421	38.433	28.649
	1.00	10.33						
	ATOM	419	OG	SER	46	23.221	38.819	27.993
	1.00	11.62						
30	ATOM	421	C	SER	46	23.556	36.106	28.484
	1.00	9.38						
	ATOM	422	O	SER	46	24.219	35.472	27.660
	1.00	9.60						
	ATOM	423	N	PRO	47	22.232	35.919	28.641
	1.00	9.69						
35	ATOM	424	CD	PRO	47	21.363	36.467	29.703
	1.00	9.98						
	ATOM	425	CA	PRO	47	21.500	34.985	27.788
	1.00	9.60						
40	ATOM	426	CB	PRO	47	20.190	34.774	28.559
	1.00	10.20						
	ATOM	427	CG	PRO	47	19.978	36.084	29.224
	1.00	10.28						
	ATOM	428	C	PRO	47	21.264	35.599	26.395
	1.00	9.80						
45	ATOM	429	O	PRO	47	20.771	34.915	25.492
	1.00	10.61						
	ATOM	430	N	PHE	48	21.644	36.872	26.223
	1.00	8.32						
50	ATOM	432	CA	PHE	48	21.461	37.576	24.949
	1.00	8.97						
	ATOM	433	CB	PHE	48	20.830	38.952	25.189
	1.00	10.54						
	ATOM	434	CG	PHE	48	19.587	38.903	26.020
	1.00	12.40						
55	ATOM	435	CD1	PHE	48	18.507	38.142	25.610
	1.00	14.30						

	ATOM	436	CD2	PHE	48	19.527	39.558	27.239
	1.00	14.43						
	ATOM	437	CE1	PHE	48	17.379	38.028	26.410
	1.00	15.31						
5	ATOM	438	CE2	PHE	48	18.400	39.448	28.043
	1.00	14.37						
	ATOM	439	CZ	PHE	48	17.332	38.683	27.627
	1.00	14.77						
	ATOM	440	C	PHE	48	22.751	37.772	24.154
10	1.00	9.38						
	ATOM	441	O	PHE	48	22.724	38.313	23.054
	1.00	9.35						
	ATOM	442	N	ARG	49	23.876	37.324	24.699
	1.00	8.82						
15	ATOM	444	CA	ARG	49	25.152	37.512	24.019
	1.00	8.97						
	ATOM	445	CB	ARG	49	26.306	37.267	24.992
	1.00	9.78						
	ATOM	446	CG	ARG	49	27.663	37.691	24.421
20	1.00	10.95						
	ATOM	447	CD	ARG	49	28.794	37.437	25.386
	1.00	12.16						
	ATOM	448	NE	ARG	49	28.529	37.971	26.716
	1.00	17.17						
25	ATOM	450	CZ	ARG	49	28.663	39.245	27.065
	1.00	16.53						
	ATOM	451	NH1	ARG	49	29.062	40.153	26.188
	1.00	19.05						
	ATOM	454	NH2	ARG	49	28.418	39.606	28.314
30	1.00	18.90						
	ATOM	457	C	ARG	49	25.349	36.630	22.800
	1.00	7.49						
	ATOM	458	O	ARG	49	24.889	35.491	22.773
	1.00	8.16						
35	ATOM	459	N	THR	50	25.986	37.184	21.772
	1.00	7.58						
	ATOM	461	CA	THR	50	26.325	36.426	20.574
	1.00	8.69						
	ATOM	462	CB	THR	50	25.873	37.143	19.293
40	1.00	9.20						
	ATOM	463	OG1	THR	50	24.453	37.318	19.334
	1.00	10.54						
	ATOM	465	CG2	THR	50	26.236	36.330	18.071
	1.00	10.59						
45	ATOM	466	C	THR	50	27.849	36.345	20.636
	1.00	9.39						
	ATOM	467	O	THR	50	28.535	37.373	20.662
	1.00	10.80						
	ATOM	468	N	ILE	51	28.358	35.128	20.762
50	1.00	8.53						
	ATOM	470	CA	ILE	51	29.789	34.895	20.881
	1.00	9.68						
	ATOM	471	CB	ILE	51	30.074	33.748	21.897
	1.00	9.85						
55	ATOM	472	CG2	ILE	51	31.567	33.462	21.984
	1.00	11.72						

	ATOM	473	CG1	ILE	51	29.548	34.118	23.297
	1.00	11.54						
	ATOM	474	CD1	ILE	51	28.097	33.689	23.565
	1.00	11.67						
5	ATOM	475	C	ILE	51	30.422	34.577	19.535
	1.00	9.84						
	ATOM	476	O	ILE	51	29.891	33.784	18.753
	1.00	9.89						
10	ATOM	477	N	ASN	52	31.541	35.231	19.252
	1.00	9.72						
	ATOM	479	CA	ASN	52	32.265	35.007	18.002
	1.00	9.63						
	ATOM	480	CB	ASN	52	32.512	36.323	17.268
	1.00	12.27						
15	ATOM	481	CG	ASN	52	31.239	37.060	16.956
	1.00	16.92						
	ATOM	482	OD1	ASN	52	30.579	36.770	15.960
	1.00	20.42						
	ATOM	483	ND2	ASN	52	30.869	38.004	17.817
20	1.00	18.67						
	ATOM	486	C	ASN	52	33.618	34.430	18.359
	1.00	8.99						
	ATOM	487	O	ASN	52	34.216	34.813	19.369
	1.00	8.30						
25	ATOM	488	N	TYR	53	34.101	33.502	17.546
	1.00	8.54						
	ATOM	490	CA	TYR	53	35.417	32.938	17.805
	1.00	8.38						
	ATOM	491	CB	TYR	53	35.383	31.888	18.931
30	1.00	8.90						
	ATOM	492	CG	TYR	53	34.816	30.545	18.510
	1.00	8.55						
	ATOM	493	CD1	TYR	53	35.652	29.541	18.013
	1.00	8.13						
35	ATOM	494	CE1	TYR	53	35.142	28.318	17.595
	1.00	7.11						
	ATOM	495	CD2	TYR	53	33.446	30.286	18.582
	1.00	8.30						
	ATOM	496	CE2	TYR	53	32.924	29.062	18.164
40	1.00	7.39						
	ATOM	497	CZ	TYR	53	33.771	28.085	17.670
	1.00	7.17						
	ATOM	498	OH	TYR	53	33.270	26.875	17.235
	1.00	8.09						
45	ATOM	500	C	TYR	53	35.995	32.333	16.549
	1.00	8.13						
	ATOM	501	O	TYR	53	35.289	32.095	15.567
	1.00	8.60						
	ATOM	502	N	ASN	54	37.305	32.146	16.568
50	1.00	7.89						
	ATOM	504	CA	ASN	54	38.011	31.525	15.466
	1.00	8.58						
	ATOM	505	CB	ASN	54	38.628	32.583	14.532
	1.00	8.69						
55	ATOM	506	CG	ASN	54	39.273	31.967	13.291
	1.00	9.70						

	ATOM	507	OD1	ASN	54	39.001	32.391	12.157
	1.00	11.48						
	ATOM	508	ND2	ASN	54	40.133	30.989	13.490
	1.00	8.91						
5	ATOM	511	C	ASN	54	39.106	30.705	16.137
	1.00	8.10						
	ATOM	512	O	ASN	54	39.984	31.262	16.807
	1.00	7.97						
10	ATOM	513	N	ALA	55	39.010	29.386	16.031
	1.00	7.16						
	ATOM	515	CA	ALA	55	40.028	28.510	16.607
	1.00	8.25						
	ATOM	516	CB	ALA	55	39.406	27.201	17.109
	1.00	9.23						
15	ATOM	517	C	ALA	55	41.090	28.235	15.529
	1.00	9.13						
	ATOM	518	O	ALA	55	40.897	27.380	14.656
	1.00	9.17						
20	ATOM	519	N	GLY	56	42.176	29.000	15.569
	1.00	9.32						
	ATOM	521	CA	GLY	56	43.254	28.829	14.606
	1.00	10.02						
	ATOM	522	C	GLY	56	43.912	27.459	14.705
	1.00	11.23						
25	ATOM	523	O	GLY	56	44.430	26.928	13.716
	1.00	11.91						
	ATOM	524	N	VAL	57	43.933	26.900	15.910
	1.00	9.79						
30	ATOM	526	CA	VAL	57	44.483	25.572	16.150
	1.00	9.61						
	ATOM	527	CB	VAL	57	45.869	25.628	16.856
	1.00	10.77						
	ATOM	528	CG1	VAL	57	46.378	24.211	17.158
	1.00	10.95						
35	ATOM	529	CG2	VAL	57	46.873	26.378	15.998
	1.00	12.00						
	ATOM	530	C	VAL	57	43.530	24.837	17.086
	1.00	9.35						
40	ATOM	531	O	VAL	57	43.121	25.388	18.118
	1.00	8.73						
	ATOM	532	N	TRP	58	43.104	23.644	16.682
	1.00	9.21						
	ATOM	534	CA	TRP	58	42.258	22.797	17.520
	1.00	9.14						
45	ATOM	535	CB	TRP	58	40.771	22.855	17.137
	1.00	8.81						
	ATOM	536	CG	TRP	58	39.950	21.927	17.984
	1.00	8.75						
50	ATOM	537	CD2	TRP	58	39.906	21.883	19.421
	1.00	8.67						
	ATOM	538	CE2	TRP	58	39.101	20.778	19.781
	1.00	9.27						
	ATOM	539	CE3	TRP	58	40.478	22.662	20.434
	1.00	8.89						
55	ATOM	540	CD1	TRP	58	39.177	20.883	17.550
	1.00	9.50						

	ATOM	541	NE1	TRP	58	38.670	20.189	18.620
	1.00	10.22						
	ATOM	543	CZ2	TRP	58	38.854	20.434	21.113
	1.00	9.53						
5	ATOM	544	CZ3	TRP	58	40.234	22.321	21.756
	1.00	9.53						
	ATOM	545	CH2	TRP	58	39.428	21.214	22.083
	1.00	10.28						
10	ATOM	546	C	TRP	58	42.841	21.418	17.283
	1.00	9.95						
	ATOM	547	O	TRP	58	42.496	20.741	16.323
	1.00	10.38						
	ATOM	548	N	ALA	59	43.732	21.011	18.177
	1.00	9.50						
15	ATOM	550	CA	ALA	59	44.443	19.750	18.031
	1.00	10.62						
	ATOM	551	CB	ALA	59	45.850	20.038	17.520
	1.00	11.24						
20	ATOM	552	C	ALA	59	44.503	18.893	19.295
	1.00	11.50						
	ATOM	553	O	ALA	59	45.574	18.702	19.893
	1.00	11.67						
	ATOM	554	N	PRO	60	43.345	18.417	19.763
	1.00	11.64						
25	ATOM	555	CD	PRO	60	41.964	18.696	19.313
	1.00	12.34						
	ATOM	556	CA	PRO	60	43.355	17.582	20.963
	1.00	12.06						
30	ATOM	557	CB	PRO	60	41.878	17.587	21.386
	1.00	12.35						
	ATOM	558	CG	PRO	60	41.157	17.657	20.069
	1.00	12.25						
	ATOM	559	C	PRO	60	43.827	16.165	20.610
	1.00	13.28						
35	ATOM	560	O	PRO	60	43.472	15.638	19.559
	1.00	14.06						
	ATOM	561	N	ASN	61	44.655	15.580	21.470
	1.00	13.72						
40	ATOM	563	CA	ASN	61	45.150	14.208	21.309
	1.00	16.04						
	ATOM	564	CB	ASN	61	46.663	14.142	21.519
	1.00	17.34						
	ATOM	565	CG	ASN	61	47.422	14.081	20.239
	1.00	19.52						
45	ATOM	566	OD1	ASN	61	46.846	14.130	19.159
	1.00	22.18						
	ATOM	567	ND2	ASN	61	48.733	13.960	20.342
	1.00	21.75						
50	ATOM	570	C	ASN	61	44.502	13.396	22.418
	1.00	17.14						
	ATOM	571	O	ASN	61	45.193	12.805	23.265
	1.00	20.86						
	ATOM	572	N	GLY	62	43.181	13.442	22.478
	1.00	14.28						
55	ATOM	574	CA	GLY	62	42.460	12.724	23.505
	1.00	12.24						

	ATOM	575	C	GLY	62	41.195	13.489	23.824
	1.00	11.02						
	ATOM	576	O	GLY	62	40.695	14.229	22.976
	1.00	11.20						
5	ATOM	577	N	ASN	63	40.733	13.379	25.064
	1.00	9.94						
	ATOM	579	CA	ASN	63	39.501	14.033	25.508
	1.00	9.74						
	ATOM	580	CB	ASN	63	38.994	13.326	26.769
10	1.00	11.20						
	ATOM	581	CG	ASN	63	37.598	13.776	27.201
	1.00	12.59						
	ATOM	582	OD1	ASN	63	37.040	13.221	28.147
	1.00	17.15						
15	ATOM	583	ND2	ASN	63	37.033	14.768	26.529
	1.00	13.79						
	ATOM	586	C	ASN	63	39.673	15.531	25.764
	1.00	9.16						
	ATOM	587	O	ASN	63	40.365	15.937	26.697
20	1.00	9.76						
	ATOM	588	N	GLY	64	39.040	16.339	24.919
	1.00	8.41						
	ATOM	590	CA	GLY	64	39.092	17.787	25.045
	1.00	8.11						
25	ATOM	591	C	GLY	64	37.887	18.376	24.327
	1.00	7.55						
	ATOM	592	O	GLY	64	37.430	17.794	23.339
	1.00	7.74						
	ATOM	593	N	TYR	65	37.366	19.496	24.830
30	1.00	7.16						
	ATOM	595	CA	TYR	65	36.198	20.172	24.242
	1.00	5.64						
	ATOM	596	CB	TYR	65	35.032	20.281	25.249
	1.00	6.56						
35	ATOM	597	CG	TYR	65	34.628	19.022	25.992
	1.00	8.02						
	ATOM	598	CD1	TYR	65	34.618	17.780	25.369
	1.00	8.25						
	ATOM	599	CE1	TYR	65	34.220	16.645	26.048
40	1.00	9.23						
	ATOM	600	CD2	TYR	65	34.222	19.090	27.324
	1.00	8.95						
	ATOM	601	CE2	TYR	65	33.816	17.959	28.012
	1.00	9.90						
45	ATOM	602	CZ	TYR	65	33.817	16.739	27.370
	1.00	10.73						
	ATOM	603	OH	TYR	65	33.412	15.599	28.045
	1.00	12.55						
	ATOM	605	C	TYR	65	36.520	21.619	23.866
50	1.00	6.29						
	ATOM	606	O	TYR	65	37.244	22.316	24.588
	1.00	7.00						
	ATOM	607	N	LEU	66	35.970	22.063	22.743
	1.00	5.38						
55	ATOM	609	CA	LEU	66	36.083	23.445	22.283
	1.00	5.78						

	ATOM	610	CB	LEU	66	36.442	23.495	20.799
	1.00	7.24						
	ATOM	611	CG	LEU	66	36.461	24.907	20.208
	1.00	7.92						
5	ATOM	612	CD1	LEU	66	37.475	25.780	20.976
	1.00	10.09						
	ATOM	613	CD2	LEU	66	36.803	24.829	18.727
	1.00	9.90						
10	ATOM	614	C	LEU	66	34.622	23.830	22.525
	1.00	6.54						
	ATOM	615	O	LEU	66	33.722	23.435	21.758
	1.00	5.88						
	ATOM	616	N	THR	67	34.389	24.653	23.542
	1.00	6.32						
15	ATOM	618	CA	THR	67	33.017	24.899	23.964
	1.00	6.62						
	ATOM	619	CB	THR	67	32.687	23.771	25.014
	1.00	5.96						
20	ATOM	620	OG1	THR	67	31.338	23.878	25.482
	1.00	6.25						
	ATOM	622	CG2	THR	67	33.641	23.834	26.239
	1.00	6.12						
	ATOM	623	C	THR	67	32.757	26.231	24.650
	1.00	5.91						
25	ATOM	624	O	THR	67	33.651	26.792	25.281
	1.00	5.87						
	ATOM	625	N	LEU	68	31.541	26.756	24.496
	1.00	5.49						
30	ATOM	627	CA	LEU	68	31.141	27.950	25.232
	1.00	5.70						
	ATOM	628	CB	LEU	68	29.806	28.488	24.741
	1.00	7.05						
	ATOM	629	CG	LEU	68	29.314	29.725	25.491
	1.00	8.06						
35	ATOM	630	CD1	LEU	68	30.210	30.922	25.209
	1.00	10.31						
	ATOM	631	CD2	LEU	68	27.874	30.009	25.092
	1.00	10.13						
40	ATOM	632	C	LEU	68	30.961	27.334	26.626
	1.00	6.24						
	ATOM	633	O	LEU	68	30.436	26.212	26.765
	1.00	6.15						
	ATOM	634	N	TYR	69	31.357	28.062	27.656
	1.00	5.92						
45	ATOM	636	CA	TYR	69	31.323	27.516	28.997
	1.00	6.43						
	ATOM	637	CB	TYR	69	32.733	26.961	29.292
	1.00	7.92						
50	ATOM	638	CG	TYR	69	32.942	26.431	30.685
	1.00	7.81						
	ATOM	639	CD1	TYR	69	32.482	25.170	31.039
	1.00	8.51						
	ATOM	640	CE1	TYR	69	32.650	24.689	32.315
	1.00	9.90						
55	ATOM	641	CD2	TYR	69	33.586	27.199	31.652
	1.00	8.54						

	ATOM	642	CE2	TYR	69	33.756	26.727	32.931
	1.00	8.83						
	ATOM	643	CZ	TYR	69	33.282	25.472	33.258
	1.00	8.64						
5	ATOM	644	OH	TYR	69	33.410	25.015	34.551
	1.00	10.08						
	ATOM	646	C	TYR	69	30.964	28.601	29.989
	1.00	6.66						
	ATOM	647	O	TYR	69	31.456	29.723	29.898
10	1.00	6.52						
	ATOM	648	N	GLY	70	30.119	28.274	30.957
	1.00	5.93						
	ATOM	650	CA	GLY	70	29.770	29.283	31.935
	1.00	7.20						
15	ATOM	651	C	GLY	70	29.001	28.724	33.108
	1.00	6.61						
	ATOM	652	O	GLY	70	28.698	27.530	33.167
	1.00	6.24						
	ATOM	653	N	TRP	71	28.699	29.602	34.054
20	1.00	7.21						
	ATOM	655	CA	TRP	71	27.953	29.215	35.240
	1.00	7.25						
	ATOM	656	CB	TRP	71	28.865	29.170	36.478
	1.00	8.08						
25	ATOM	657	CG	TRP	71	29.887	28.097	36.524
	1.00	9.15						
	ATOM	658	CD2	TRP	71	29.803	26.869	37.253
	1.00	9.01						
	ATOM	659	CE2	TRP	71	31.016	26.176	37.049
30	1.00	9.87						
	ATOM	660	CE3	TRP	71	28.818	26.283	38.057
	1.00	10.02						
	ATOM	661	CD1	TRP	71	31.112	28.106	35.920
	1.00	8.19						
35	ATOM	662	NE1	TRP	71	31.793	26.952	36.228
	1.00	9.71						
	ATOM	664	CZ2	TRP	71	31.271	24.925	37.621
	1.00	10.26						
	ATOM	665	CZ3	TRP	71	29.068	25.043	38.621
40	1.00	11.63						
	ATOM	666	CH2	TRP	71	30.286	24.375	38.401
	1.00	11.11						
	ATOM	667	C	TRP	71	26.893	30.220	35.620
	1.00	7.86						
45	ATOM	668	O	TRP	71	26.976	31.401	35.273
	1.00	7.90						
	ATOM	669	N	THR	72	25.895	29.725	36.340
	1.00	9.00						
	ATOM	671	CA	THR	72	24.907	30.593	36.960
50	1.00	9.70						
	ATOM	672	CB	THR	72	23.473	30.521	36.379
	1.00	10.06						
	ATOM	673	OG1	THR	72	22.939	29.204	36.544
	1.00	10.75						
55	ATOM	675	CG2	THR	72	23.431	30.955	34.929
	1.00	9.49						



	ATOM	676	C	THR	72	24.837	30.066	38.389
	1.00	11.21						
	ATOM	677	O	THR	72	25.246	28.926	38.670
	1.00	10.30						
5	ATOM	678	N	ARG	73	24.362	30.914	39.289
	1.00	13.21						
	ATOM	680	CA	ARG	73	24.156	30.555	40.687
	1.00	15.05						
10	ATOM	681	CB	ARG	73	24.932	31.488	41.621
	1.00	16.77						
	ATOM	682	CG	ARG	73	26.430	31.290	41.596
	1.00	18.20						
	ATOM	683	CD	ARG	73	27.103	32.107	42.682
	1.00	19.22						
15	ATOM	684	NE	ARG	73	28.538	31.835	42.766
	1.00	21.45						
	ATOM	686	CZ	ARG	73	29.466	32.495	42.079
	1.00	22.40						
20	ATOM	687	NH1	ARG	73	29.118	33.465	41.247
	1.00	24.34						
	ATOM	690	NH2	ARG	73	30.748	32.209	42.247
	1.00	23.90						
	ATOM	693	C	ARG	73	22.658	30.745	40.901
	1.00	15.76						
25	ATOM	694	O	ARG	73	22.001	31.435	40.114
	1.00	15.54						
	ATOM	695	N	SER	74	22.125	30.124	41.949
	1.00	17.09						
30	ATOM	697	CA	SER	74	20.701	30.215	42.283
	1.00	18.69						
	ATOM	698	CB	SER	74	20.370	31.620	42.798
	1.00	19.69						
	ATOM	699	OG	SER	74	21.282	31.998	43.817
	1.00	24.14						
35	ATOM	701	C	SER	74	19.759	29.838	41.126
	1.00	17.91						
	ATOM	702	O	SER	74	18.998	30.673	40.625
	1.00	18.35						
40	ATOM	703	N	PRO	75	19.793	28.572	40.693
	1.00	17.77						
	ATOM	704	CD	PRO	75	18.753	28.012	39.810
	1.00	18.55						
	ATOM	705	CA	PRO	75	20.653	27.508	41.224
	1.00	17.24						
45	ATOM	706	CB	PRO	75	19.828	26.253	40.969
	1.00	18.06						
	ATOM	707	CG	PRO	75	19.175	26.565	39.666
	1.00	18.68						
50	ATOM	708	C	PRO	75	21.999	27.423	40.515
	1.00	16.14						
	ATOM	709	O	PRO	75	22.231	28.081	39.492
	1.00	15.03						
	ATOM	710	N	LEU	76	22.875	26.608	41.080
	1.00	14.58						
55	ATOM	712	CA	LEU	76	24.207	26.389	40.547
	1.00	14.02						

	ATOM	713	CB	LEU	76	25.063	25.722	41.623
	1.00	16.02						
	ATOM	714	CG	LEU	76	26.575	25.774	41.487
	1.00	18.13						
5	ATOM	715	CD1	LEU	76	27.047	27.219	41.526
	1.00	18.22						
	ATOM	716	CD2	LEU	76	27.197	24.970	42.626
	1.00	18.98						
	ATOM	717	C	LEU	76	24.112	25.488	39.312
10	1.00	12.79						
	ATOM	718	O	LEU	76	23.722	24.323	39.412
	1.00	12.48						
	ATOM	719	N	ILE	77	24.482	26.025	38.151
	1.00	11.37						
15	ATOM	721	CA	ILE	77	24.431	25.266	36.902
	1.00	10.64						
	ATOM	722	CB	ILE	77	23.188	25.655	36.054
	1.00	11.91						
	ATOM	723	CG2	ILE	77	23.253	24.994	34.686
20	1.00	11.77						
	ATOM	724	CG1	ILE	77	21.898	25.234	36.769
	1.00	12.91						
	ATOM	725	CD1	ILE	77	20.656	25.787	36.160
	1.00	14.88						
25	ATOM	726	C	ILE	77	25.676	25.555	36.068
	1.00	8.64						
	ATOM	727	O	ILE	77	26.084	26.712	35.948
	1.00	8.92						
	ATOM	728	N	GLU	78	26.319	24.502	35.574
30	1.00	7.66						
	ATOM	730	CA	GLU	78	27.503	24.621	34.720
	1.00	7.21						
	ATOM	731	CB	GLU	78	28.536	23.573	35.134
	1.00	7.73						
35	ATOM	732	CG	GLU	78	29.868	23.635	34.372
	1.00	9.08						
	ATOM	733	CD	GLU	78	30.835	22.544	34.805
	1.00	10.20						
	ATOM	734	OE1	GLU	78	32.050	22.814	34.932
40	1.00	10.78						
	ATOM	735	OE2	GLU	78	30.395	21.407	35.026
	1.00	10.70						
	ATOM	736	C	GLU	78	26.961	24.315	33.322
	1.00	7.93						
45	ATOM	737	O	GLU	78	26.391	23.240	33.112
	1.00	9.13						
	ATOM	738	N	TYR	79	27.119	25.229	32.369
	1.00	7.30						
	ATOM	740	CA	TYR	79	26.562	24.982	31.046
50	1.00	6.18						
	ATOM	741	CB	TYR	79	25.422	25.963	30.737
	1.00	6.50						
	ATOM	742	CG	TYR	79	25.844	27.414	30.631
	1.00	6.96						
55	ATOM	743	CD1	TYR	79	26.466	27.896	29.479
	1.00	6.30						

	ATOM	744	CE1	TYR	79	26.861	29.215	29.376
	1.00	7.02						
	ATOM	745	CD2	TYR	79	25.626	28.299	31.681
	1.00	7.12						
5	ATOM	746	CE2	TYR	79	26.019	29.633	31.584
	1.00	7.44						
	ATOM	747	CZ	TYR	79	26.636	30.079	30.427
	1.00	7.25						
10	ATOM	748	OH	TYR	79	27.042	31.388	30.303
	1.00	8.96						
	ATOM	750	C	TYR	79	27.605	24.969	29.939
	1.00	7.01						
	ATOM	751	O	TYR	79	28.658	25.619	30.044
	1.00	5.99						
15	ATOM	752	N	TYR	80	27.235	24.315	28.840
	1.00	6.31						
	ATOM	754	CA	TYR	80	28.112	24.128	27.692
	1.00	5.86						
	ATOM	755	CB	TYR	80	28.667	22.695	27.722
20	1.00	5.72						
	ATOM	756	CG	TYR	80	29.620	22.352	28.827
	1.00	5.27						
	ATOM	757	CD1	TYR	80	29.159	21.881	30.055
	1.00	7.53						
25	ATOM	758	CE1	TYR	80	30.042	21.465	31.032
	1.00	7.89						
	ATOM	759	CD2	TYR	80	30.983	22.403	28.608
	1.00	7.64						
	ATOM	760	CE2	TYR	80	31.865	21.995	29.566
30	1.00	8.52						
	ATOM	761	CZ	TYR	80	31.394	21.523	30.776
	1.00	9.81						
	ATOM	762	OH	TYR	80	32.297	21.100	31.725
	1.00	10.19						
35	ATOM	764	C	TYR	80	27.413	24.207	26.346
	1.00	6.25						
	ATOM	765	O	TYR	80	26.268	23.762	26.216
	1.00	6.36						
	ATOM	766	N	VAL	81	28.111	24.755	25.354
40	1.00	5.60						
	ATOM	768	CA	VAL	81	27.650	24.709	23.956
	1.00	4.96						
	ATOM	769	CB	VAL	81	27.189	26.044	23.369
	1.00	6.50						
45	ATOM	770	CG1	VAL	81	26.812	25.814	21.903
	1.00	6.96						
	ATOM	771	CG2	VAL	81	25.955	26.567	24.133
	1.00	7.32						
	ATOM	772	C	VAL	81	28.915	24.204	23.252
50	1.00	5.73						
	ATOM	773	O	VAL	81	29.854	24.963	22.970
	1.00	5.99						
	ATOM	774	N	VAL	82	28.957	22.897	23.048
	1.00	4.96						
55	ATOM	776	CA	VAL	82	30.123	22.242	22.470
	1.00	5.85						

	ATOM	777	CB	VAL	82	30.246	20.785	23.010
	1.00	5.93						
	ATOM	778	CG1	VAL	82	31.540	20.140	22.517
	1.00	7.63						
5	ATOM	779	CG2	VAL	82	30.205	20.766	24.539
	1.00	6.83						
	ATOM	780	C	VAL	82	30.119	22.221	20.951
	1.00	6.61						
	ATOM	781	O	VAL	82	29.261	21.582	20.348
10	1.00	6.74						
	ATOM	782	N	ASP	83	31.119	22.864	20.340
	1.00	6.11						
	ATOM	784	CA	ASP	83	31.237	22.909	18.874
	1.00	6.12						
15	ATOM	785	CB	ASP	83	31.679	24.290	18.395
	1.00	5.67						
	ATOM	786	CG	ASP	83	30.504	25.196	18.052
	1.00	6.35						
	ATOM	787	OD1	ASP	83	30.737	26.382	17.772
20	1.00	7.42						
	ATOM	788	OD2	ASP	83	29.350	24.720	18.044
	1.00	7.63						
	ATOM	789	C	ASP	83	32.160	21.835	18.312
	1.00	6.63						
25	ATOM	790	O	ASP	83	31.995	21.399	17.175
	1.00	7.51						
	ATOM	791	N	SER	84	33.188	21.479	19.069
	1.00	6.29						
	ATOM	793	CA	SER	84	34.085	20.424	18.641
30	1.00	6.74						
	ATOM	794	CB	SER	84	35.198	20.933	17.727
	1.00	6.37						
	ATOM	795	OG	SER	84	35.909	19.816	17.225
	1.00	6.88						
35	ATOM	797	C	SER	84	34.655	19.706	19.851
	1.00	6.53						
	ATOM	798	O	SER	84	34.527	20.167	20.988
	1.00	6.69						
	ATOM	799	N	TRP	85	35.236	18.545	19.606
40	1.00	6.77						
	ATOM	801	CA	TRP	85	35.780	17.732	20.675
	1.00	7.16						
	ATOM	802	CB	TRP	85	34.667	16.856	21.276
	1.00	7.31						
45	ATOM	803	CG	TRP	85	33.955	15.981	20.279
	1.00	8.40						
	ATOM	804	CD2	TRP	85	32.790	16.319	19.504
	1.00	8.19						
	ATOM	805	CE2	TRP	85	32.500	15.209	18.683
50	1.00	8.37						
	ATOM	806	CE3	TRP	85	31.970	17.449	19.425
	1.00	8.60						
	ATOM	807	CD1	TRP	85	34.303	14.711	19.911
	1.00	9.75						
55	ATOM	808	NE1	TRP	85	33.434	14.243	18.950
	1.00	10.01						

	ATOM	810	CZ2	TRP	85	31.428	15.198	17.793
	1.00	8.41						
	ATOM	811	CZ3	TRP	85	30.905	17.432	18.537
	1.00	9.35						
5	ATOM	812	CH2	TRP	85	30.649	16.313	17.737
	1.00	9.03						
	ATOM	813	C	TRP	85	36.914	16.881	20.127
	1.00	8.11						
10	ATOM	814	O	TRP	85	37.254	16.976	18.939
	1.00	8.43						
	ATOM	815	N	GLY	86	37.518	16.094	21.006
	1.00	8.18						
	ATOM	817	CA	GLY	86	38.603	15.225	20.609
	1.00	8.41						
15	ATOM	818	C	GLY	86	38.137	13.815	20.335
	1.00	9.11						
	ATOM	819	O	GLY	86	37.402	13.561	19.381
	1.00	10.63						
20	ATOM	820	N	THR	87	38.534	12.895	21.197
	1.00	9.04						
	ATOM	822	CA	THR	87	38.185	11.491	21.029
	1.00	10.41						
	ATOM	823	CB	THR	87	39.277	10.586	21.643
	1.00	10.21						
25	ATOM	824	OG1	THR	87	39.518	10.996	22.996
	1.00	12.01						
	ATOM	826	CG2	THR	87	40.579	10.676	20.842
	1.00	11.49						
	ATOM	827	C	THR	87	36.852	11.086	21.637
30	1.00	11.00						
	ATOM	828	O	THR	87	36.345	9.997	21.350
	1.00	12.97						
	ATOM	829	N	TYR	88	36.286	11.949	22.473
	1.00	11.01						
35	ATOM	831	CA	TYR	88	35.033	11.641	23.165
	1.00	11.59						
	ATOM	832	CB	TYR	88	35.323	11.459	24.669
	1.00	12.77						
	ATOM	833	CG	TYR	88	34.096	11.360	25.553
40	1.00	15.23						
	ATOM	834	CD1	TYR	88	33.282	10.236	25.521
	1.00	17.59						
	ATOM	835	CE1	TYR	88	32.116	10.177	26.273
	1.00	18.52						
45	ATOM	836	CD2	TYR	88	33.720	12.419	26.372
	1.00	16.34						
	ATOM	837	CE2	TYR	88	32.566	12.368	27.127
	1.00	17.85						
	ATOM	838	CZ	TYR	88	31.763	11.250	27.071
50	1.00	19.24						
	ATOM	839	OH	TYR	88	30.583	11.222	27.789
	1.00	21.51						
	ATOM	841	C	TYR	88	33.970	12.713	22.981
	1.00	10.42						
55	ATOM	842	O	TYR	88	34.211	13.886	23.290
	1.00	9.91						

	ATOM	843	N	ARG	89	32.812	12.325	22.450
	1.00	10.21						
	ATOM	845	CA	ARG	89	31.717	13.277	22.278
	1.00	9.91						
5	ATOM	846	CB	ARG	89	30.852	12.918	21.063
	1.00	9.65						
	ATOM	847	CG	ARG	89	29.751	13.920	20.805
	1.00	8.70						
	ATOM	848	CD	ARG	89	28.867	13.540	19.623
10	1.00	8.30						
	ATOM	849	NE	ARG	89	27.824	14.550	19.439
	1.00	8.00						
	ATOM	851	CZ	ARG	89	26.565	14.414	19.857
	1.00	7.35						
15	ATOM	852	NH1	ARG	89	26.170	13.300	20.460
	1.00	8.01						
	ATOM	855	NH2	ARG	89	25.729	15.435	19.750
	1.00	8.94						
	ATOM	858	C	ARG	89	30.886	13.218	23.563
20	1.00	9.57						
	ATOM	859	O	ARG	89	30.381	12.157	23.936
	1.00	9.70						
	ATOM	860	N	PRO	90	30.766	14.348	24.276
	1.00	9.28						
25	ATOM	861	CD	PRO	90	31.298	15.695	23.987
	1.00	10.13						
	ATOM	862	CA	PRO	90	29.984	14.337	25.514
	1.00	10.21						
	ATOM	863	CB	PRO	90	30.311	15.695	26.139
30	1.00	10.53						
	ATOM	864	CG	PRO	90	30.543	16.570	24.965
	1.00	10.45						
	ATOM	865	C	PRO	90	28.486	14.136	25.294
	1.00	11.31						
35	ATOM	866	O	PRO	90	27.890	14.725	24.385
	1.00	12.21						
	ATOM	867	N	THR	91	27.890	13.263	26.096
	1.00	10.98						
	ATOM	869	CA	THR	91	26.459	13.001	25.995
40	1.00	13.17						
	ATOM	870	CB	THR	91	26.144	11.723	25.167
	1.00	13.69						
	ATOM	871	OG1	THR	91	26.655	10.563	25.841
	1.00	16.21						
45	ATOM	873	CG2	THR	91	26.757	11.814	23.754
	1.00	13.50						
	ATOM	874	C	THR	91	25.885	12.875	27.406
	1.00	13.53						
	ATOM	875	O	THR	91	26.626	12.903	28.392
50	1.00	15.22						
	ATOM	876	N	GLY	92	24.566	12.783	27.505
	1.00	12.71						
	ATOM	878	CA	GLY	92	23.915	12.659	28.798
	1.00	12.21						
55	ATOM	879	C	GLY	92	22.488	12.240	28.541
	1.00	12.62						

	ATOM	880	O	GLY	92	22.232	11.459	27.617
	1.00	12.73						
	ATOM	881	N	THR	93	21.558	12.754	29.343
	1.00	11.34						
5	ATOM	883	CA	THR	93	20.143	12.442	29.175
	1.00	12.11						
	ATOM	884	CB	THR	93	19.380	12.724	30.480
	1.00	13.13						
10	ATOM	885	OG1	THR	93	19.941	11.922	31.528
	1.00	14.32						
	ATOM	887	CG2	THR	93	17.897	12.397	30.328
	1.00	14.22						
	ATOM	888	C	THR	93	19.606	13.311	28.039
	1.00	10.68						
15	ATOM	889	O	THR	93	19.596	14.538	28.139
	1.00	10.38						
	ATOM	890	N	TYR	94	19.191	12.668	26.951
	1.00	10.81						
20	ATOM	892	CA	TYR	94	18.691	13.369	25.775
	1.00	10.59						
	ATOM	893	CB	TYR	94	18.532	12.381	24.619
	1.00	11.92						
	ATOM	894	CG	TYR	94	18.014	13.008	23.347
	1.00	11.53						
25	ATOM	895	CD1	TYR	94	.00	8.59	
	ATOM	964	CG	ASP	101	24.966	30.278	15.615
	1.00	9.23						
	ATOM	965	OD1	ASP	101	24.632	29.849	16.740
	1.00	8.01						
30	ATOM	966	OD2	ASP	101	24.891	31.481	15.300
	1.00	11.33						
	ATOM	967	C	ASP	101	24.872	27.940	12.547
	1.00	10.53						
	ATOM	968	O	ASP	101	26.063	27.625	12.533
35	1.00	11.20						
	ATOM	969	N	GLY	102	23.957	27.394	11.746
	1.00	10.95						
	ATOM	971	CA	GLY	102	24.323	26.415	10.740
	1.00	11.74						
40	ATOM	972	C	GLY	102	24.522	24.991	11.203
	1.00	12.03						
	ATOM	973	O	GLY	102	24.849	24.130	10.387
	1.00	15.13						
	ATOM	974	N	GLY	103	24.331	24.720	12.489
45	1.00	10.73						
	ATOM	976	CA	GLY	103	24.520	23.366	12.968
	1.00	9.93						
	ATOM	977	C	GLY	103	23.331	22.865	13.753
	1.00	8.93						
50	ATOM	978	O	GLY	103	22.442	23.643	14.096
	1.00	9.85						
	ATOM	979	N	THR	104	23.272	21.554	13.952
	1.00	8.69						
	ATOM	981	CA	THR	104	22.207	20.950	14.753
55	1.00	8.72						



	ATOM	982	CB	THR	104	21.513	19.802	14.014
	1.00	10.36						
	ATOM	983	OG1	THR	104	20.972	20.313	12.788
	1.00	13.06						
5	ATOM	985	CG2	THR	104	20.379	19.211	14.873
	1.00	10.48						
	ATOM	986	C	THR	104	22.887	20.429	16.020
	1.00	8.40						
	ATOM	987	O	THR	104	23.919	19.741	15.948
10	1.00	8.43						
	ATOM	988	N	TYR	105	22.312	20.766	17.167
	1.00	6.69						
	ATOM	990	CA	TYR	105	22.869	20.382	18.453
	1.00	7.22						
15	ATOM	991	CB	TYR	105	23.138	21.636	19.296
	1.00	6.90						
	ATOM	992	CG	TYR	105	24.168	22.602	18.740
	1.00	7.17						
	ATOM	993	CD1	TYR	105	23.853	23.459	17.693
20	1.00	7.56						
	ATOM	994	CE1	TYR	105	24.777	24.367	17.210
	1.00	7.90						
	ATOM	995	CD2	TYR	105	25.447	22.677	19.292
	1.00	6.18						
25	ATOM	996	CE2	TYR	105	26.379	23.585	18.818
	1.00	7.32						
	ATOM	997	CZ	TYR	105	26.036	24.425	17.779
	1.00	7.75						
	ATOM	998	OH	TYR	105	26.940	25.358	17.306
30	1.00	8.32						
	ATOM	1000	C	TYR	105	21.907	19.505	19.240
	1.00	7.65						
	ATOM	1001	O	TYR	105	20.703	19.742	19.233
	1.00	8.32						
35	ATOM	1002	N	ASP	106	22.436	18.470	19.877
	1.00	7.03						
	ATOM	1004	CA	ASP	106	21.621	17.629	20.744
	1.00	7.19						
	ATOM	1005	CB	ASP	106	22.232	16.242	20.895
40	1.00	7.44						
	ATOM	1006	CG	ASP	106	22.135	15.434	19.635
	1.00	8.29						
	ATOM	1007	OD1	ASP	106	23.134	14.788	19.269
	1.00	8.93						
45	ATOM	1008	OD2	ASP	106	21.051	15.468	19.011
	1.00	8.87						
	ATOM	1009	C	ASP	106	21.650	18.319	22.100
	1.00	6.52						
	ATOM	1010	O	ASP	106	22.678	18.897	22.489
50	1.00	8.85						
	ATOM	1011	N	ILE	107	20.545	18.254	22.830
	1.00	6.54						
	ATOM	1013	CA	ILE	107	20.456	18.862	24.154
	1.00	7.09						
55	ATOM	1014	CB	ILE	107	19.151	19.675	24.297
	1.00	7.73						

	ATOM	1015	CG2	ILE	107	19.023	20.234	25.710
	1.00	6.87						
	ATOM	1016	CG1	ILE	107	19.117	20.790	23.249
	1.00	8.04						
5	ATOM	1017	CD1	ILE	107	17.748	21.473	23.124
	1.00	9.19						
	ATOM	1018	C	ILE	107	20.491	17.755	25.205
	1.00	7.06						
10	ATOM	1019	O	ILE	107	19.722	16.789	25.123
	1.00	7.22						
	ATOM	1020	N	TYR	108	21.389	17.880	26.173
	1.00	6.95						
	ATOM	1022	CA	TYR	108	21.515	16.882	27.232
	1.00	7.18						
15	ATOM	1023	CB	TYR	108	22.811	16.077	27.090
	1.00	7.59						
	ATOM	1024	CG	TYR	108	23.013	15.341	25.794
	1.00	8.26						
20	ATOM	1025	CD1	TYR	108	23.988	15.753	24.887
	1.00	8.13						
	ATOM	1026	CE1	TYR	108	24.213	15.060	23.719
	1.00	8.60						
	ATOM	1027	CD2	TYR	108	22.267	14.208	25.493
	1.00	8.68						
25	ATOM	1028	CE2	TYR	108	22.486	13.502	24.324
	1.00	8.88						
	ATOM	1029	CZ	TYR	108	23.458	13.933	23.441
	1.00	9.66						
30	ATOM	1030	OH	TYR	108	23.681	13.242	22.276
	1.00	9.55						
	ATOM	1032	C	TYR	108	21.617	17.506	28.607
	1.00	7.18						
	ATOM	1033	O	TYR	108	22.041	18.662	28.748
	1.00	6.50						
35	ATOM	1034	N	THR	109	21.259	16.721	29.620
	1.00	7.71						
	ATOM	1036	CA	THR	109	21.465	17.144	31.003
	1.00	8.74						
40	ATOM	1037	CB	THR	109	20.173	17.372	31.831
	1.00	9.86						
	ATOM	1038	OG1	THR	109	19.393	16.169	31.862
	1.00	11.56						
	ATOM	1040	CG2	THR	109	19.371	18.521	31.276
	1.00	12.46						
45	ATOM	1041	C	THR	109	22.241	16.028	31.670
	1.00	8.80						
	ATOM	1042	O	THR	109	22.121	14.849	31.295
	1.00	8.91						
50	ATOM	1043	N	THR	110	23.095	16.412	32.606
	1.00	8.78						
	ATOM	1045	CA	THR	110	23.876	15.470	33.401
	1.00	10.13						
	ATOM	1046	CB	THR	110	25.327	15.244	32.854
	1.00	10.63						
55	ATOM	1047	OG1	THR	110	26.021	16.493	32.771
	1.00	10.44						

	ATOM	1049	CG2	THR	110	25.316	14.558	31.483
	1.00	10.74						
	ATOM	1050	C	THR	110	23.972	16.094	34.792
	1.00	9.98						
5	ATOM	1051	O	THR	110	23.632	17.264	34.990
	1.00	10.66						
	ATOM	1052	N	THR	111	24.451	15.312	35.747
	1.00	10.72						
10	ATOM	1054	CA	THR	111	24.620	15.777	37.114
	1.00	11.19						
	ATOM	1055	CB	THR	111	23.582	15.125	38.047
	1.00	13.02						
	ATOM	1056	OG1	THR	111	22.270	15.388	37.539
	1.00	15.05						
15	ATOM	1058	CG2	THR	111	23.695	15.684	39.476
	1.00	13.84						
	ATOM	1059	C	THR	111	26.015	15.372	37.566
	1.00	11.62						
	ATOM	1060	O	THR	111	26.505	14.306	37.199
20	1.00	11.90						
	ATOM	1061	N	ARG	112	26.674	16.269	38.290
	1.00	10.81						
	ATOM	1063	CA	ARG	112	28.002	16.016	38.839
	1.00	11.90						
25	ATOM	1064	CB	ARG	112	28.930	17.201	38.558
	1.00	14.38						
	ATOM	1065	CG	ARG	112	29.291	17.330	37.103
	1.00	16.14						
	ATOM	1066	CD	ARG	112	30.426	16.404	36.731
30	1.00	19.66						
	ATOM	1067	NE	ARG	112	31.707	17.057	36.981
	1.00	23.60						
	ATOM	1069	CZ	ARG	112	32.767	16.477	37.542
	1.00	25.66						
35	ATOM	1070	NH1	ARG	112	32.724	15.204	37.927
	1.00	27.05						
	ATOM	1073	NH2	ARG	112	33.867	17.193	37.756
	1.00	27.17						
	ATOM	1076	C	ARG	112	27.819	15.843	40.344
40	1.00	11.36						
	ATOM	1077	O	ARG	112	27.071	16.595	40.978
	1.00	11.70						
	ATOM	1078	N	TYR	113	28.465	14.829	40.900
	1.00	11.50						
45	ATOM	1080	CA	TYR	113	28.366	14.530	42.323
	1.00	12.45						
	ATOM	1081	CB	TYR	113	27.883	13.090	42.519
	1.00	12.53						
	ATOM	1082	CG	TYR	113	26.550	12.818	41.855
50	1.00	13.06						
	ATOM	1083	CD1	TYR	113	25.356	13.014	42.547
	1.00	13.72						
	ATOM	1084	CE1	TYR	113	24.139	12.792	41.945
	1.00	13.98						
55	ATOM	1085	CD2	TYR	113	26.489	12.389	40.536
	1.00	13.33						

	ATOM	1086	CE2	TYR	113	25.267	12.162	39.920
	1.00	13.75						
	ATOM	1087	CZ	TYR	113	24.099	12.365	40.635
	1.00	13.86						
5	ATOM	1088	OH	TYR	113	22.884	12.113	40.036
	1.00	15.43						
	ATOM	1090	C	TYR	113	29.702	14.724	43.032
	1.00	13.26						
10	ATOM	1091	O	TYR	113	30.718	14.139	42.625
	1.00	13.92						
	ATOM	1092	N	ASN	114	29.678	15.537	44.088
	1.00	13.07						
	ATOM	1094	CA	ASN	114	30.861	15.840	44.901
	1.00	12.98						
15	ATOM	1095	CB	ASN	114	31.251	14.610	45.723
	1.00	14.43						
	ATOM	1096	CG	ASN	114	32.206	14.942	46.855
	1.00	15.38						
20	ATOM	1097	OD1	ASN	114	32.035	15.938	47.562
	1.00	17.02						
	ATOM	1098	ND2	ASN	114	33.191	14.085	47.057
	1.00	17.49						
	ATOM	1101	C	ASN	114	32.017	16.274	44.000
	1.00	13.11						
25	ATOM	1102	O	ASN	114	33.127	15.736	44.073
	1.00	13.52						
	ATOM	1103	N	ALA	115	31.743	17.264	43.162
	1.00	11.72						
	ATOM	1105	CA	ALA	115	32.726	17.764	42.208
30	1.00	11.90						
	ATOM	1106	CB	ALA	115	32.176	17.594	40.786
	1.00	12.69						
	ATOM	1107	C	ALA	115	33.037	19.231	42.471
	1.00	11.91						
35	ATOM	1108	O	ALA	115	32.214	19.955	43.039
	1.00	11.60						
	ATOM	1109	N	PRO	116	34.232	19.693	42.055
	1.00	12.08						
40	ATOM	1110	CD	PRO	116	35.306	18.936	41.388
	1.00	12.97						
	ATOM	1111	CA	PRO	116	34.619	21.092	42.258
	1.00	12.75						
	ATOM	1112	CB	PRO	116	36.022	21.158	41.642
	1.00	13.29						
45	ATOM	1113	CG	PRO	116	36.525	19.757	41.718
	1.00	14.85						
	ATOM	1114	C	PRO	116	33.666	22.013	41.496
	1.00	13.38						
	ATOM	1115	O	PRO	116	33.319	21.745	40.339
50	1.00	13.48						
	ATOM	1116	N	SER	117	33.228	23.084	42.142
	1.00	13.65						
	ATOM	1118	CA	SER	117	32.339	24.019	41.482
	1.00	14.63						
55	ATOM	1119	CB	SER	117	31.012	24.124	42.231
	1.00	15.34						

	ATOM	1120	OG	SER	117	31.158	24.930	43.385
	1.00	17.33						
	ATOM	1122	C	SER	117	33.022	25.379	41.436
	1.00	14.80						
5	ATOM	1123	O	SER	117	34.129	25.553	41.960
	1.00	14.72						
	ATOM	1124	N	ILE	118	32.328	26.348	40.853
	1.00	14.62						
10	ATOM	1126	CA	ILE	118	32.837	27.703	40.728
	1.00	16.31						
	ATOM	1127	CB	ILE	118	31.813	28.600	39.976
	1.00	15.37						
	ATOM	1128	CG2	ILE	118	30.488	28.670	40.731
	1.00	14.25						
15	ATOM	1129	CG1	ILE	118	32.392	29.993	39.741
	1.00	16.02						
	ATOM	1130	CD1	ILE	118	31.520	30.875	38.868
	1.00	16.65						
20	ATOM	1131	C	ILE	118	33.206	28.321	42.080
	1.00	17.92						
	ATOM	1132	O	ILE	118	34.183	29.055	42.174
	1.00	18.87						
	ATOM	1133	N	ASP	119	32.455	27.974	43.123
	1.00	20.29						
25	ATOM	1135	CA	ASP	119	32.674	28.507	44.472
	1.00	22.48						
	ATOM	1136	CB	ASP	119	31.415	28.308	45.327
	1.00	24.91						
30	ATOM	1137	CG	ASP	119	30.283	29.248	44.952
	1.00	26.95						
	ATOM	1138	OD1	ASP	119	30.568	30.400	44.566
	1.00	27.78						
	ATOM	1139	OD2	ASP	119	29.106	28.830	45.071
	1.00	29.45						
35	ATOM	1140	C	ASP	119	33.834	27.866	45.226
	1.00	23.22						
	ATOM	1141	O	ASP	119	34.165	28.300	46.339
	1.00	24.26						
40	ATOM	1142	N	GLY	120	34.450	26.844	44.640
	1.00	21.95						
	ATOM	1144	CA	GLY	120	35.519	26.148	45.332
	1.00	21.06						
	ATOM	1145	C	GLY	120	34.867	24.995	46.081
	1.00	20.24						
45	ATOM	1146	O	GLY	120	33.639	24.838	46.041
	1.00	21.54						
	ATOM	1147	N	ASP	121	35.663	24.198	46.780
	1.00	18.87						
	ATOM	1149	CA	ASP	121	35.151	23.043	47.515
50	1.00	17.79						
	ATOM	1150	CB	ASP	121	34.292	23.489	48.709
	1.00	16.14						
	ATOM	1151	CG	ASP	121	35.128	24.177	49.781
	1.00	16.04						
55	ATOM	1152	OD1	ASP	121	36.279	23.733	49.983
	1.00	16.20						

	ATOM	1153	OD2	ASP	121	34.660	25.169	50.381
	1.00	15.66						
	ATOM	1154	C	ASP	121	34.431	22.078	46.565
	1.00	17.56						
5	ATOM	1155	O	ASP	121	34.707	22.097	45.360
	1.00	20.27						
	ATOM	1156	N	ARG	122	33.541	21.233	47.071
	1.00	15.49						
10	ATOM	1158	CA	ARG	122	32.868	20.264	46.211
	1.00	14.33						
	ATOM	1159	CB	ARG	122	33.468	18.871	46.417
	1.00	15.98						
	ATOM	1160	CG	ARG	122	34.987	18.856	46.370
	1.00	22.01						
15	ATOM	1161	CD	ARG	122	35.555	17.493	46.647
	1.00	25.64						
	ATOM	1162	NE	ARG	122	35.516	16.674	45.446
	1.00	30.29						
20	ATOM	1164	CZ	ARG	122	36.541	15.960	44.996
	1.00	32.24						
	ATOM	1165	NH1	ARG	122	37.699	15.959	45.650
	1.00	33.69						
	ATOM	1168	NH2	ARG	122	36.411	15.255	43.880
	1.00	34.20						
25	ATOM	1171	C	ARG	122	31.386	20.210	46.513
	1.00	12.98						
	ATOM	1172	O	ARG	122	30.978	20.389	47.657
	1.00	13.04						
30	ATOM	1173	N	THR	123	30.579	19.961	45.492
	1.00	11.93						
	ATOM	1175	CA	THR	123	29.144	19.878	45.705
	1.00	11.52						
	ATOM	1176	CB	THR	123	28.517	21.287	45.856
	1.00	12.34						
35	ATOM	1177	OG1	THR	123	27.219	21.171	46.455
	1.00	13.52						
	ATOM	1179	CG2	THR	123	28.408	22.004	44.503
	1.00	12.64						
40	ATOM	1180	C	THR	123	28.507	19.108	44.558
	1.00	11.60						
	ATOM	1181	O	THR	123	29.212	18.577	43.694
	1.00	12.00						
	ATOM	1182	N	THR	124	27.187	18.988	44.592
	1.00	10.11						
45	ATOM	1184	CA	THR	124	26.451	18.283	43.548
	1.00	11.46						
	ATOM	1185	CB	THR	124	25.470	17.273	44.172
	1.00	11.44						
	ATOM	1186	OG1	THR	124	26.212	16.222	44.818
50	1.00	13.54						
	ATOM	1188	CG2	THR	124	24.564	16.679	43.105
	1.00	12.97						
	ATOM	1189	C	THR	124	25.691	19.343	42.738
	1.00	11.64						
55	ATOM	1190	O	THR	124	25.013	20.201	43.307
	1.00	12.44						

	ATOM	1191	N	PHE	125	25.841	19.321	41.420
	1.00	10.02						
	ATOM	1193	CA	PHE	125	25.172	20.310	40.581
	1.00	9.87						
5	ATOM	1194	CB	PHE	125	26.040	21.581	40.430
	1.00	10.39						
	ATOM	1195	CG	PHE	125	27.430	21.321	39.899
	1.00	10.80						
10	ATOM	1196	CD1	PHE	125	28.486	21.072	40.771
	1.00	10.51						
	ATOM	1197	CD2	PHE	125	27.681	21.298	38.526
	1.00	10.72						
	ATOM	1198	CE1	PHE	125	29.760	20.801	40.290
	1.00	10.49						
15	ATOM	1199	CE2	PHE	125	28.956	21.027	38.037
	1.00	11.56						
	ATOM	1200	CZ	PHE	125	29.991	20.779	38.911
	1.00	10.93						
20	ATOM	1201	C	PHE	125	24.813	19.744	39.216
	1.00	9.17						
	ATOM	1202	O	PHE	125	25.350	18.720	38.791
	1.00	9.91						
	ATOM	1203	N	THR	126	23.886	20.418	38.547
	1.00	9.93						
25	ATOM	1205	CA	THR	126	23.431	20.026	37.222
	1.00	10.19						
	ATOM	1206	CB	THR	126	21.949	20.388	37.041
	1.00	13.09						
30	ATOM	1207	OG1	THR	126	21.192	19.813	38.113
	1.00	15.71						
	ATOM	1209	CG2	THR	126	21.416	19.847	35.715
	1.00	15.34						
	ATOM	1210	C	THR	126	24.223	20.729	36.122
	1.00	9.09						
35	ATOM	1211	O	THR	126	24.701	21.857	36.305
	1.00	9.18						
	ATOM	1212	N	GLN	127	24.389	20.028	35.005
	1.00	8.52						
40	ATOM	1214	CA	GLN	127	25.075	20.560	33.832
	1.00	7.83						
	ATOM	1215	CB	GLN	127	26.264	19.683	33.444
	1.00	7.94						
	ATOM	1216	CG	GLN	127	27.314	19.489	34.527
	1.00	8.42						
45	ATOM	1217	CD	GLN	127	28.410	18.547	34.080
	1.00	9.41						
	ATOM	1218	OE1	GLN	127	28.173	17.364	33.849
	1.00	11.46						
50	ATOM	1219	NE2	GLN	127	29.599	19.072	33.903
	1.00	9.24						
	ATOM	1222	C	GLN	127	24.082	20.546	32.671
	1.00	8.00						
	ATOM	1223	O	GLN	127	23.335	19.570	32.500
	1.00	9.01						
55	ATOM	1224	N	TYR	128	24.050	21.637	31.915
	1.00	7.47						

	ATOM	1226	CA	TYR	128	23.193	21.747	30.725
	1.00	7.08						
	ATOM	1227	CB	TYR	128	22.446	23.076	30.678
	1.00	7.17						
5	ATOM	1228	CG	TYR	128	21.337	23.250	31.683
	1.00	7.55						
	ATOM	1229	CD1	TYR	128	20.883	22.185	32.458
	1.00	8.48						
10	ATOM	1230	CE1	TYR	128	19.866	22.370	33.389
	1.00	9.54						
	ATOM	1231	CD2	TYR	128	20.748	24.495	31.859
	1.00	8.26						
	ATOM	1232	CE2	TYR	128	19.737	24.686	32.784
	1.00	8.94						
15	ATOM	1233	CZ	TYR	128	19.304	23.625	33.543
	1.00	8.68						
	ATOM	1234	OH	TYR	128	18.303	23.828	34.475
	1.00	10.00						
	ATOM	1236	C	TYR	128	24.143	21.720	29.539
20	1.00	6.99						
	ATOM	1237	O	TYR	128	25.161	22.422	29.550
	1.00	7.10						
	ATOM	1238	N	TRP	129	23.786	20.956	28.511
	1.00	6.30						
25	ATOM	1240	CA	TRP	129	24.626	20.849	27.320
	1.00	6.02						
	ATOM	1241	CB	TRP	129	25.266	19.455	27.203
	1.00	6.55						
	ATOM	1242	CG	TRP	129	26.025	18.930	28.374
30	1.00	76.122	1.00	9.09				
	ATOM	1211	O	THR	126	24.701	21.857	36.305
	1.00	9.18						
	ATOM	1212	N	GLN	127	24.389	20.028	35.005
	1.00	8.52						
35	ATOM	1214	CA	GLN	127	25.075	20.560	33.832
	1.00	7.83						
	ATOM	1215	CB	GLN	127	26.264	19.683	33.444
	1.00	7.94						
	ATOM	1216	CG	GLN	127	27.314	19.489	34.527
40	1.00	8.42						
	ATOM	1217	CD	GLN	127	28.410	18.547	34.080
	1.00	9.41						
	ATOM	1218	OE1	GLN	127	28.173	17.364	33.849
	1.00	11.46						
45	ATOM	1219	NE2	GLN	127	29.599	19.072	33.903
	1.00	9.24						
	ATOM	1222	C	GLN	127	24.082	20.546	32.671
	1.00	8.00						
	ATOM	1223	O	GLN	127	23.335	19.570	32.500
50	1.00	9.01						
	ATOM	1224	N	TYR	128	24.050	21.637	31.915
	1.00	7.47						
	ATOM	1226	CA	TYR	128	23.193	21.747	30.725
	1.00	7.08						
55	ATOM	1227	CB	TYR	128	22.446	23.076	30.678
	1.00	7.17						

	ATOM	1228	CG	TYR	128	21.337	23.250	31.683
	1.00	7.55						
	ATOM	1229	CD1	TYR	128	20.883	22.185	32.458
	1.00	8.48						
5	ATOM	1230	CE1	TYR	128	19.866	22.370	33.389
	1.00	9.54						
	ATOM	1231	CD2	TYR	128	20.748	24.495	31.859
	1.00	8.26						
10	ATOM	1232	CE2	TYR	128	19.737	24.686	32.784
	1.00	8.94						
	ATOM	1233	CZ	TYR	128	19.304	23.625	33.543
	1.00	8.68						
	ATOM	1234	OH	TYR	128	18.303	23.828	34.475
	1.00	10.00						
15	ATOM	1236	C	TYR	128	24.143	21.720	29.539
	1.00	6.99						
	ATOM	1237	O	TYR	128	25.161	22.422	29.550
	1.00	7.10						
20	ATOM	1238	N	TRP	129	23.786	20.956	28.511
	1.00	6.30						
	ATOM	1240	CA	TRP	129	24.626	20.849	27.320
	1.00	6.02						
	ATOM	1241	CB	TRP	129	25.266	19.455	27.203
	1.00	6.55						
25	ATOM	1242	CG	TRP	129	26.025	18.930	28.374
	1.00	7.49						
	ATOM	1243	CD2	TRP	129	27.451	18.787	28.477
	1.00	7.83						
30	ATOM	1244	CE2	TRP	129	27.722	18.209	29.731
	1.00	8.17						
	ATOM	1245	CE3	TRP	129	28.522	19.086	27.622
	1.00	7.59						
	ATOM	1246	CD1	TRP	129	25.506	18.444	29.541
	1.00	8.08						
35	ATOM	1247	NE1	TRP	129	26.517	18.009	30.362
	1.00	8.78						
	ATOM	1249	CZ2	TRP	129	29.028	17.921	30.156
	1.00	8.09						
40	ATOM	1250	CZ3	TRP	129	29.806	18.797	28.044
	1.00	7.89						
	ATOM	1251	CH2	TRP	129	30.049	18.221	29.297
	1.00	8.85						
	ATOM	1252	C	TRP	129	23.879	20.976	26.010
	1.00	6.91						
45	ATOM	1253	O	TRP	129	22.750	20.503	25.891
	1.00	6.88						
	ATOM	1254	N	SER	130	24.532	21.630	25.051
	1.00	6.19						
50	ATOM	1256	CA	SER	130	24.101	21.652	23.655
	1.00	5.86						
	ATOM	1257	CB	SER	130	23.813	23.049	23.120
	1.00	7.32						
	ATOM	1258	OG	SER	130	22.470	23.416	23.404
	1.00	7.36						
55	ATOM	1260	C	SER	130	25.385	21.110	23.022
	1.00	5.75						

	ATOM	1261	O	SER	130	26.447	21.723	23.188
	1.00	7.07						
	ATOM	1262	N	VAL	131	25.313	19.945	22.387
	1.00	5.14						
5	ATOM	1264	CA	VAL	131	26.490	19.328	21.762
	1.00	6.25						
	ATOM	1265	CB	VAL	131	26.797	17.953	22.401
	1.00	6.01						
10	ATOM	1266	CG1	VAL	131	28.104	17.379	21.836
	1.00	7.33						
	ATOM	1267	CG2	VAL	131	26.910	18.089	23.913
	1.00	8.18						
	ATOM	1268	C	VAL	131	26.230	19.155	20.269
	1.00	6.01						
15	ATOM	1269	O	VAL	131	25.270	18.491	19.868
	1.00	7.09						
	ATOM	1270	N	ARG	132	27.075	19.755	19.433
	1.00	6.07						
20	ATOM	1272	CA	ARG	132	26.877	19.667	17.989
	1.00	5.80						
	ATOM	1273	CB	ARG	132	27.971	20.447	17.262
	1.00	6.74						
	ATOM	1274	CG	ARG	132	27.492	21.119	15.982
	1.00	7.33						
25	ATOM	1275	CD	ARG	132	28.601	22.044	15.465
	1.00	7.95						
	ATOM	1276	NE	ARG	132	28.257	22.750	14.230
	1.00	10.15						
30	ATOM	1278	CZ	ARG	132	28.405	22.248	13.007
	1.00	9.87						
	ATOM	1279	NH1	ARG	132	28.883	21.020	12.830
	1.00	9.74						
	ATOM	1282	NH2	ARG	132	28.098	22.993	11.956
	1.00	11.62						
35	ATOM	1285	C	ARG	132	26.867	18.194	17.560
	1.00	5.99						
	ATOM	1286	O	ARG	132	27.605	17.374	18.110
	1.00	6.38						
40	ATOM	1287	N	GLN	133	26.022	17.849	16.590
	1.00	7.04						
	ATOM	1289	CA	GLN	133	25.941	16.457	16.156
	1.00	7.51						
	ATOM	1290	CB	GLN	133	24.677	16.213	15.328
	1.00	8.04						
45	ATOM	1291	CG	GLN	133	23.402	16.324	16.174
	1.00	8.11						
	ATOM	1292	CD	GLN	133	22.125	15.987	15.413
	1.00	9.11						
50	ATOM	1293	OE1	GLN	133	21.084	15.701	16.022
	1.00	12.22						
	ATOM	1294	NE2	GLN	133	22.193	16.014	14.095
	1.00	8.08						
	ATOM	1297	C	GLN	133	27.191	15.996	15.421
	1.00	7.25						
55	ATOM	1298	O	GLN	133	27.554	14.821	15.497
	1.00	8.01						

	ATOM	1299	N	SER	134	27.830	16.927	14.713
	1.00	7.38						
	ATOM	1301	CA	SER	134	29.084	16.677	13.986
	1.00	8.47						
5	ATOM	1302	CB	SER	134	28.839	16.670	12.467
	1.00	10.32						
	ATOM	1303	OG	SER	134	28.295	17.904	12.025
	1.00	11.99						
10	ATOM	1305	C	SER	134	30.024	17.825	14.382
	1.00	8.30						
	ATOM	1306	O	SER	134	29.552	18.911	14.738
	1.00	7.97						
	ATOM	1307	N	LYS	135	31.336	17.588	14.353
	1.00	7.49						
15	ATOM	1309	CA	LYS	135	32.288	18.633	14.722
	1.00	7.91						
	ATOM	1310	CB	LYS	135	33.733	18.098	14.730
	1.00	7.88						
20	ATOM	1311	CG	LYS	135	33.968	16.992	15.737
	1.00	9.26						
	ATOM	1312	CD	LYS	135	35.408	16.520	15.771
	1.00	10.17						
	ATOM	1313	CE	LYS	135	35.552	15.304	16.668
	1.00	10.79						
25	ATOM	1314	NZ	LYS	135	36.989	14.926	16.843
	1.00	13.41						
	ATOM	1318	C	LYS	135	32.217	19.823	13.783
	1.00	8.47						
30	ATOM	1319	O	LYS	135	32.134	19.664	12.554
	1.00	10.44						
	ATOM	1320	N	ARG	136	32.239	21.023	14.353
	1.00	8.73						
	ATOM	1322	CA	ARG	136	32.227	22.225	13.548
	1.00	8.79						
35	ATOM	1323	CB	ARG	136	31.842	23.431	14.397
	1.00	8.71						
	ATOM	1324	CG	ARG	136	31.469	24.661	13.597
	1.00	8.96						
40	ATOM	1325	CD	ARG	136	30.960	25.755	14.519
	1.00	8.67						
	ATOM	1326	NE	ARG	136	30.367	26.877	13.797
	1.00	8.17						
	ATOM	1328	CZ	ARG	136	29.614	27.817	14.361
	1.00	7.64						
45	ATOM	1329	NH1	ARG	136	29.354	27.777	15.661
	1.00	8.13						
	ATOM	1332	NH2	ARG	136	29.121	28.807	13.631
	1.00	8.82						
50	ATOM	1335	C	ARG	136	33.650	22.412	13.027
	1.00	9.51						
	ATOM	1336	O	ARG	136	34.609	22.278	13.785
	1.00	9.99						
	ATOM	1337	N	PRO	137	33.810	22.679	11.720
	1.00	10.43						
55	ATOM	1338	CD	PRO	137	32.814	22.730	10.637
	1.00	10.71						

	ATOM	1339	CA	PRO	137	35.172	22.877	11.193
	1.00	11.19						
	ATOM	1340	CB	PRO	137	34.916	23.225	9.728
	1.00	12.07						
5	ATOM	1341	CG	PRO	137	33.665	22.488	9.420
	1.00	11.96						
	ATOM	1342	C	PRO	137	35.810	24.072	11.917
	1.00	10.74						
10	ATOM	1343	O	PRO	137	35.110	25.007	12.320
	1.00	12.54						
	ATOM	1344	N	THR	138	37.114	24.023	12.139
	1.00	10.87						
	ATOM	1346	CA	THR	138	37.795	25.116	12.811
	1.00	11.05						
15	ATOM	1347	CB	THR	138	38.652	24.604	13.982
	1.00	11.69						
	ATOM	1348	OG1	THR	138	39.583	23.616	13.512
	1.00	12.49						
20	ATOM	1350	CG2	THR	138	37.746	24.000	15.070
	1.00	11.85						
	ATOM	1351	C	THR	138	38.650	25.904	11.826
	1.00	10.93						
	ATOM	1352	O	THR	138	38.816	25.493	10.675
	1.00	12.46						
25	ATOM	1353	N	GLY	139	39.132	27.061	12.259
	1.00	10.76						
	ATOM	1355	CA	GLY	139	39.954	27.889	11.397
	1.00	11.16						
30	ATOM	1356	C	GLY	139	39.157	29.004	10.743
	1.00	12.00						
	ATOM	1357	O	GLY	139	39.730	29.873	10.085
	1.00	14.10						
	ATOM	1358	N	SER	140	37.839	28.981	10.930
	1.00	11.25						
35	ATOM	1360	CA	SER	140	36.954	29.996	10.375
	1.00	11.51						
	ATOM	1361	CB	SER	140	35.857	29.343	9.538
	1.00	13.27						
40	ATOM	1362	OG	SER	140	36.404	28.701	8.403
	1.00	17.64						
	ATOM	1364	C	SER	140	36.293	30.823	11.468
	1.00	9.96						
	ATOM	1365	O	SER	140	36.369	30.485	12.657
	1.00	10.71						
45	ATOM	1366	N	ASN	141	35.697	31.937	11.064
	1.00	9.76						
	ATOM	1368	CA	ASN	141	34.988	32.815	11.988
	1.00	10.29						
50	ATOM	1369	CB	ASN	141	34.774	34.193	11.357
	1.00	11.11						
	ATOM	1370	CG	ASN	141	36.068	34.965	11.187
	1.00	12.89						
	ATOM	1371	OD1	ASN	141	37.056	34.714	11.885
	1.00	11.87						
55	ATOM	1372	ND2	ASN	141	36.066	35.914	10.270
	1.00	14.96						

	ATOM	1375	C	ASN	141	33.645	32.158	12.283
	1.00	10.47						
	ATOM	1376	O	ASN	141	32.787	32.050	11.399
	1.00	11.70						
5	ATOM	1377	N	ALA	142	33.477	31.712	13.523
	1.00	9.61						
	ATOM	1379	CA	ALA	142	32.265	31.022	13.945
	1.00	9.98						
	ATOM	1380	CB	ALA	142	32.629	29.707	14.600
10	1.00	9.88						
	ATOM	1381	C	ALA	142	31.457	31.875	14.903
	1.00	10.25						
	ATOM	1382	O	ALA	142	32.001	32.719	15.618
	1.00	11.29						
15	ATOM	1383	N	THR	143	30.155	31.627	14.927
	1.00	9.82						
	ATOM	1385	CA	THR	143	29.246	32.357	15.788
	1.00	9.36						
	ATOM	1386	CB	THR	143	28.277	33.232	14.953
20	1.00	11.22						
	ATOM	1387	OG1	THR	143	29.033	34.077	14.069
	1.00	14.26						
	ATOM	1389	CG2	THR	143	27.412	34.092	15.847
	1.00	12.93						
25	ATOM	1390	C	THR	143	28.389	31.394	16.596
	1.00	9.04						
	ATOM	1391	O	THR	143	28.011	30.319	16.114
	1.00	8.71						
	ATOM	1392	N	ILE	144	28.179	31.740	17.859
30	1.00	7.22						
	ATOM	1394	CA	ILE	144	27.297	30.977	18.725
	1.00	7.94						
	ATOM	1395	CB	ILE	144	28.030	30.341	19.930
	1.00	7.57						
35	ATOM	1396	CG2	ILE	144	26.998	29.785	20.946
	1.00	8.85						
	ATOM	1397	CG1	ILE	144	28.951	29.218	19.445
	1.00	8.51						
	ATOM	1398	CD1	ILE	144	29.793	28.590	20.549
40	1.00	8.96						
	ATOM	1399	C	ILE	144	26.262	31.992	19.213
	1.00	7.28						
	ATOM	1400	O	ILE	144	26.592	32.926	19.951
	1.00	7.79						
45	ATOM	1401	N	THR	145	25.033	31.857	18.721
	1.00	7.04						
	ATOM	1403	CA	THR	145	23.929	32.739	19.102
	1.00	7.58						
	ATOM	1404	CB	THR	145	22.930	32.837	17.950
50	1.00	7.57						
	ATOM	1405	OG1	THR	145	23.616	33.323	16.786
	1.00	9.20						
	ATOM	1407	CG2	THR	145	21.813	33.805	18.295
	1.00	9.33						
55	ATOM	1408	C	THR	145	23.331	32.077	20.345
	1.00	7.68						

	ATOM	1409	O	THR	145	22.444	31.214	20.262
	1.00	7.61						
	ATOM	1410	N	PHE	146	23.861	32.470	21.500
	1.00	7.43						
5	ATOM	1412	CA	PHE	146	23.486	31.856	22.761
	1.00	7.32						
	ATOM	1413	CB	PHE	146	24.361	32.297	23.893
	1.00	7.88						
10	ATOM	1414	CG	PHE	146	24.232	31.635	25.189
	1.00	7.47						
	ATOM	1415	CD1	PHE	146	24.328	30.247	25.221
	1.00	8.42						
	ATOM	1416	CD2	PHE	146	24.032	32.318	26.380
	1.00	9.10						
15	ATOM	1417	CE1	PHE	146	24.231	29.560	26.429
	1.00	10.17						
	ATOM	1418	CE2	PHE	146	23.934	31.636	27.589
	1.00	9.57						
	ATOM	1419	CZ	PHE	146	24.034	30.259	27.611
20	1.00	9.43						
	ATOM	1420	C	PHE	146	22.016	31.897	23.106
	1.00	7.62						
	ATOM	1421	O	PHE	146	21.493	30.937	23.682
	1.00	7.42						
25	ATOM	1422	N	THR	147	21.330	32.950	22.677
	1.00	7.24						
	ATOM	1424	CA	THR	147	19.907	33.059	22.958
	1.00	8.68						
	ATOM	1425	CB	THR	147	19.331	34.382	22.419
30	1.00	9.43						
	ATOM	1426	OG1	THR	147	17.947	34.473	22.777
	1.00	17.10						
	ATOM	1428	CG2	THR	147	19.433	34.429	20.930
	1.00	10.81						
35	ATOM	1429	C	THR	147	19.109	31.868	22.396
	1.00	8.55						
	ATOM	1430	O	THR	147	18.140	31.429	23.017
	1.00	8.97						
	ATOM	1431	N	ASN	148	19.526	31.325	21.250
40	1.00	8.27						
	ATOM	1433	CA	ASN	148	18.829	30.176	20.655
	1.00	9.32						
	ATOM	1434	CB	ASN	148	19.423	29.784	19.302
	1.00	10.43						
45	ATOM	1435	CG	ASN	148	19.127	30.791	18.202
	1.00	13.00						
	ATOM	1436	OD1	ASN	148	19.860	30.861	17.201
	1.00	15.35						
	ATOM	1437	ND2	ASN	148	18.069	31.569	18.367
50	1.00	11.66						
	ATOM	1440	C	ASN	148	18.909	28.967	21.574
	1.00	8.82						
	ATOM	1441	O	ASN	148	17.949	28.202	21.697
	1.00	9.19						
55	ATOM	1442	N	HIS	149	20.056	28.804	22.232
	1.00	8.08						

	ATOM	1444	CA	HIS	149	20.264	27.693	23.149
	1.00	7.07						
	ATOM	1445	CB	HIS	149	21.755	27.507	23.426
	1.00	6.26						
5	ATOM	1446	CG	HIS	149	22.521	27.095	22.208
	1.00	6.45						
	ATOM	1447	CD2	HIS	149	23.157	27.828	21.262
	1.00	7.33						
10	ATOM	1448	ND1	HIS	149	22.654	25.776	21.826
	1.00	7.11						
	ATOM	1450	CE1	HIS	149	23.339	25.716	20.697
	1.00	7.85						
	ATOM	1451	NE2	HIS	149	23.655	26.947	20.335
	1.00	7.63						
15	ATOM	1453	C	HIS	149	19.477	27.883	24.430
	1.00	7.20						
	ATOM	1454	O	HIS	149	18.780	26.971	24.863
	1.00	8.12						
20	ATOM	1455	N	VAL	150	19.552	29.080	25.005
	1.00	7.02						
	ATOM	1457	CA	VAL	150	18.813	29.393	26.223
	1.00	7.84						
	ATOM	1458	CB	VAL	150	19.044	30.858	26.632
	1.00	7.77						
25	ATOM	1459	CG1	VAL	150	18.131	31.239	27.801
	1.00	8.91						
	ATOM	1460	CG2	VAL	150	20.515	31.052	27.014
	1.00	8.40						
30	ATOM	1461	C	VAL	150	17.313	29.139	26.017
	1.00	8.70						
	ATOM	1462	O	VAL	150	16.661	28.489	26.848
	1.00	9.04						
	ATOM	1463	N	ASN	151	16.794	29.575	24.875
	1.00	9.29						
35	ATOM	1465	CA	ASN	151	15.379	29.396	24.577
	1.00	11.27						
	ATOM	1466	CB	ASN	151	14.967	30.276	23.397
	1.00	13.99						
	ATOM	1467	CG	ASN	151	14.954	31.754	23.767
40	1.00	17.23						
	ATOM	1468	OD1	ASN	151	14.736	32.099	24.932
	1.00	22.12						
	ATOM	1469	ND2	ASN	151	15.210	32.624	22.797
	1.00	19.31						
45	ATOM	1472	C	ASN	151	14.993	27.933	24.372
	1.00	10.65						
	ATOM	1473	O	ASN	151	13.957	27.484	24.875
	1.00	11.12						
	ATOM	1474	N	ALA	152	15.828	27.180	23.660
50	1.00	9.31						
	ATOM	1476	CA	ALA	152	15.563	25.754	23.459
	1.00	8.90						
	ATOM	1477	CB	ALA	152	16.560	25.156	22.476
	1.00	10.29						
55	ATOM	1478	C	ALA	152	15.629	25.011	24.797
	1.00	9.31						

	ATOM	1479	O	ALA	152	14.812	24.121	25.066
	1.00	9.03						
	ATOM	1480	N	TRP	153	16.589	25.372	25.642
	1.00	8.56						
5	ATOM	1482	CA	TRP	153	16.723	24.728	26.941
	1.00	8.90						
	ATOM	1483	CB	TRP	153	17.970	25.239	27.677
	1.00	8.55						
10	ATOM	1484	CG	TRP	153	19.290	24.835	27.040
	1.00	8.34						
	ATOM	1485	CD2	TRP	153	20.590	25.321	27.401
	1.00	8.15						
	ATOM	1486	CE2	TRP	153	21.528	24.676	26.560
	1.00	7.87						
15	ATOM	1487	CE3	TRP	153	21.054	26.243	28.350
	1.00	8.65						
	ATOM	1488	CD1	TRP	153	19.480	23.940	26.022
	1.00	8.62						
20	ATOM	1489	NE1	TRP	153	20.829	23.836	25.729
	1.00	8.65						
	ATOM	1491	CZ2	TRP	153	22.905	24.925	26.642
	1.00	7.85						
	ATOM	1492	CZ3	TRP	153	22.420	26.491	28.429
	1.00	8.42						
25	ATOM	1493	CH2	TRP	153	23.327	25.834	27.581
	1.00	8.96						
	ATOM	1494	C	TRP	153	15.479	25.002	27.787
	1.00	9.72						
30	ATOM	1495	O	TRP	153	14.936	24.096	28.422
	1.00	10.06						
	ATOM	1496	N	LYS	154	15.012	26.245	27.753
	1.00	10.65						
	ATOM	1498	CA	LYS	154	13.834	26.636	28.514
	1.00	12.32						
35	ATOM	1499	CB	LYS	154	13.571	28.129	28.322
	1.00	14.64						
	ATOM	1500	CG	LYS	154	12.405	28.650	29.100
	1.00	20.28						
40	ATOM	1501	CD	LYS	154	12.336	30.169	29.040
	1.00	23.54						
	ATOM	1502	CE	LYS	154	11.104	30.667	29.794
	1.00	27.22						
	ATOM	1503	NZ	LYS	154	11.069	30.150	31.208
	1.00	28.84						
45	ATOM	1507	C	LYS	154	12.620	25.803	28.091
	1.00	12.89						
	ATOM	1508	O	LYS	154	11.847	25.360	28.938
	1.00	12.44						
50	ATOM	1509	N	SER	155	12.499	25.520	26.797
	1.00	13.31						
	ATOM	1511	CA	SER	155	11.372	24.732	26.298
	1.00	14.63						
	ATOM	1512	CB	SER	155	11.358	24.706	24.770
	1.00	16.22						
55	ATOM	1513	OG	SER	155	12.315	23.786	24.267
	1.00	18.53						

	ATOM	1515	C	SER	155	11.375	23.302	26.835
	1.00	15.94						
	ATOM	1516	O	SER	155	10.352	22.612	26.796
	1.00	16.03						
5	ATOM	1517	N	HIS	156	12.530	22.847	27.316
	1.00	15.14						
	ATOM	1519	CA	HIS	156	12.653	21.502	27.865
	1.00	15.16						
	ATOM	1520	CB	HIS	156	13.846	20.777	27.243
10	1.00	16.18						
	ATOM	1521	CG	HIS	156	13.660	20.483	25.795
	1.00	17.56						
	ATOM	1522	CD2	HIS	156	12.918	19.540	25.170
	1.00	17.74						
15	ATOM	1523	ND1	HIS	156	14.220	21.251	24.799
	1.00	18.24						
	ATOM	1525	CE1	HIS	156	13.832	20.795	23.622
	1.00	17.83						
	ATOM	1526	NE2	HIS	156	13.041	19.758	23.821
20	1.00	19.83						
	ATOM	1528	C	HIS	156	12.765	21.504	29.377
	1.00	14.84						
	ATOM	1529	O	HIS	156	13.220	20.525	29.973
	1.00	15.74						
25	ATOM	1530	N	GLY	157	12.349	22.607	29.991
	1.00	13.35						
	ATOM	1532	CA	GLY	157	12.404	22.719	31.438
	1.00	13.68						
	ATOM	1533	C	GLY	157	13.801	22.895	32.022
30	1.00	13.89						
	ATOM	1534	O	GLY	157	14.016	22.658	33.204
	1.00	15.37						
	ATOM	1535	N	MET	158	14.746	23.333	31.202
	1.00	11.75						
35	ATOM	1537	CA	MET	158	16.114	23.548	31.651
	1.00	11.51						
	ATOM	1538	CB	MET	158	17.083	23.009	30.598
	1.00	9.86						
	ATOM	1539	CG	MET	158	17.075	21.493	30.479
40	1.00	9.83						
	ATOM	1540	SD	MET	158	17.768	20.929	28.919
	1.00	11.15						
	ATOM	1541	CE	MET	158	19.481	21.502	29.063
	1.00	9.64						
45	ATOM	1542	C	MET	158	16.297	25.047	31.839
	1.00	11.30						
	ATOM	1543	O	MET	158	16.681	25.756	30.915
	1.00	11.61						
	ATOM	1544	N	ASN	159	15.965	25.529	33.029
50	1.00	12.08						
	ATOM	1546	CA	ASN	159	16.067	26.948	33.337
	1.00	12.87						
	ATOM	1547	CB	ASN	159	14.883	27.387	34.197
	1.00	16.49						
55	ATOM	1548	CG	ASN	159	13.557	27.198	33.486
	1.00	18.00						

	ATOM	1549	OD1	ASN	159	12.757	26.340	33.857
	1.00	22.78						
	ATOM	1550	ND2	ASN	159	13.344	27.961	32.425
	1.00	20.94						
5	ATOM	1553	C	ASN	159	17.367	27.289	34.039
	1.00	12.90						
	ATOM	1554	O	ASN	159	17.803	26.584	34.955
	1.00	12.75						
10	ATOM	1555	N	LEU	160	17.982	28.378	33.603
	1.00	12.27						
	ATOM	1557	CA	LEU	160	19.239	28.825	34.178
	1.00	13.44						
	ATOM	1558	CB	LEU	160	19.997	29.674	33.152
	1.00	13.40						
15	ATOM	1559	CG	LEU	160	20.564	28.838	32.002
	1.00	13.30						
	ATOM	1560	CD1	LEU	160	20.954	29.739	30.855
	1.00	14.40						
20	ATOM	1561	CD2	LEU	160	21.758	28.020	32.482
	1.00	13.55						
	ATOM	1562	C	LEU	160	19.007	29.596	35.480
	1.00	14.33						
	ATOM	1563	O	LEU	160	17.882	30.024	35.763
	1.00	14.67						
25	ATOM	1564	N	GLY	161	20.060	29.740	36.278
	1.00	14.47						
	ATOM	1566	CA	GLY	161	19.953	30.465	37.529
	1.00	15.47						
30	ATOM	1567	C	GLY	161	19.784	31.954	37.290
	1.00	16.15						
	ATOM	1568	O	GLY	161	19.999	32.452	36.171
	1.00	16.60						
	ATOM	1569	N	SER	162	19.445	32.683	38.347
	1.00	17.37						
35	ATOM	1571	CA	SER	162	19.239	34.121	38.230
	1.00	17.84						
	ATOM	1572	CB	SER	162	18.170	34.576	39.223
	1.00	19.00						
40	ATOM	1573	OG	SER	162	18.500	34.145	40.530
	1.00	21.73						
	ATOM	1575	C	SER	162	20.505	34.953	38.413
	1.00	17.19						
	ATOM	1576	O	SER	162	20.538	36.123	38.041
	1.00	17.92						
45	ATOM	1577	N	ASN	163	21.541	34.362	38.995
	1.00	16.21						
	ATOM	1579	CA	ASN	163	22.784	35.087	39.219
	1.00	15.87						
50	ATOM	1580	CB	ASN	163	23.260	34.871	40.661
	1.00	19.24						
	ATOM	1581	CG	ASN	163	24.477	35.718	41.020
	1.00	23.45						
	ATOM	1582	OD1	ASN	163	25.295	35.326	41.860
	1.00	27.11						
55	ATOM	1583	ND2	ASN	163	24.590	36.894	40.410
	1.00	25.66						

	ATOM	1586	C	ASN	163	23.816	34.580	38.219
	1.00	14.67						
	ATOM	1587	O	ASN	163	24.280	33.454	38.320
	1.00	15.00						
5	ATOM	1588	N	TRP	164	24.144	35.402	37.233
	1.00	12.77						
	ATOM	1590	CA	TRP	164	25.106	35.017	36.205
	1.00	12.67						
	ATOM	1591	CB	TRP	164	24.802	35.764	9.997
10	29.674	33.152	1.00	13.40				
	ATOM	1559	CG	LEU	160	20.564	28.838	32.002
	1.00	13.30						
	ATOM	1560	CD1	LEU	160	20.954	29.739	30.855
	1.00	14.40						
15	ATOM	1561	CD2	LEU	160	21.758	28.020	32.482
	1.00	13.55						
	ATOM	1562	C	LEU	160	19.007	29.596	35.480
	1.00	14.33						
	ATOM	1563	O	LEU	160	17.882	30.024	35.763
20	1.00	14.67						
	ATOM	1564	N	GLY	161	20.060	29.740	36.278
	1.00	14.47						
	ATOM	1566	CA	GLY	161	19.953	30.465	37.529
	1.00	15.47						
25	ATOM	1567	C	GLY	161	19.784	31.954	37.290
	1.00	16.15						
	ATOM	1568	O	GLY	161	19.999	32.452	36.171
	1.00	16.60						
	ATOM	1569	N	SER	162	19.445	32.683	38.347
30	1.00	17.37						
	ATOM	1571	CA	SER	162	19.239	34.121	38.230
	1.00	17.84						
	ATOM	1572	CB	SER	162	18.170	34.576	39.223
	1.00	19.00						
35	ATOM	1573	OG	SER	162	18.500	34.145	40.530
	1.00	21.73						
	ATOM	1575	C	SER	162	20.505	34.953	38.413
	1.00	17.19						
	ATOM	1576	O	SER	162	20.538	36.123	38.041
40	1.00	17.92						
	ATOM	1577	N	ASN	163	21.541	34.362	38.995
	1.00	16.21						
	ATOM	1579	CA	ASN	163	22.784	35.087	39.219
	1.00	15.87						
45	ATOM	1580	CB	ASN	163	23.260	34.871	40.661
	1.00	19.24						
	ATOM	1581	CG	ASN	163	24.477	35.718	41.020
	1.00	23.45						
	ATOM	1582	OD1	ASN	163	25.295	35.326	41.860
50	1.00	27.11						
	ATOM	1583	ND2	ASN	163	24.590	36.894	40.410
	1.00	25.66						
	ATOM	1586	C	ASN	163	23.816	34.580	38.219
	1.00	14.67						
55	ATOM	1587	O	ASN	163	24.280	33.454	38.320
	1.00	15.00						

	ATOM	1588	N	TRP	164	24.144	35.402	37.233
	1.00	12.77						
	ATOM	1590	CA	TRP	164	25.106	35.017	36.205
	1.00	12.67						
5	ATOM	1591	CB	TRP	164	24.802	35.764	34.902
	1.00	12.97						
	ATOM	1592	CG	TRP	164	23.523	35.331	34.250
	1.00	13.93						
10	ATOM	1593	CD2	TRP	164	23.393	34.489	33.098
	1.00	13.58						
	ATOM	1594	CE2	TRP	164	22.015	34.297	32.871
	1.00	14.09						
	ATOM	1595	CE3	TRP	164	24.308	33.876	32.238
	1.00	13.32						
15	ATOM	1596	CD1	TRP	164	22.253	35.620	34.659
	1.00	15.26						
	ATOM	1597	NE1	TRP	164	21.340	34.996	33.837
	1.00	15.80						
20	ATOM	1599	CZ2	TRP	164	21.534	33.518	31.825
	1.00	14.29						
	ATOM	1600	CZ3	TRP	164	23.829	33.107	31.204
	1.00	13.95						
	ATOM	1601	CH2	TRP	164	22.456	32.932	31.004
	1.00	13.84						
25	ATOM	1602	C	TRP	164	26.576	35.218	36.569
	1.00	12.17						
	ATOM	1603	O	TRP	164	26.990	36.300	37.001
	1.00	12.76						
30	ATOM	1604	N	ALA	165	27.365	34.173	36.360
	1.00	10.88						
	ATOM	1606	CA	ALA	165	28.796	34.233	36.611
	1.00	9.93						
	ATOM	1607	CB	ALA	165	29.275	32.979	37.333
	1.00	12.00						
35	ATOM	1608	C	ALA	165	29.486	34.396	35.246
	1.00	9.94						
	ATOM	1609	O	ALA	165	28.846	34.822	34.275
	1.00	10.07						
40	ATOM	1610	N	TYR	166	30.759	34.027	35.145
	1.00	8.78						
	ATOM	1612	CA	TYR	166	31.474	34.207	33.881
	1.00	8.27						
	ATOM	1613	CB	TYR	166	32.982	34.002	34.069
	1.00	8.85						
45	ATOM	1614	CG	TYR	166	33.384	32.610	34.503
	1.00	10.16						
	ATOM	1615	CD1	TYR	166	33.438	31.567	33.588
	1.00	10.41						
50	ATOM	1616	CE1	TYR	166	33.821	30.302	33.964
	1.00	12.25						
	ATOM	1617	CD2	TYR	166	33.726	32.344	35.827
	1.00	9.77						
	ATOM	1618	CE2	TYR	166	34.111	31.073	36.220
	1.00	11.27						
55	ATOM	1619	CZ	TYR	166	34.157	30.061	35.283
	1.00	11.58						

	ATOM	1620	OH	TYR	166	34.553	28.803	35.642
	1.00	13.25						
	ATOM	1622	C	TYR	166	30.941	33.364	32.717
	1.00	8.20						
5	ATOM	1623	O	TYR	166	30.242	32.355	32.915
	1.00	8.68						
	ATOM	1624	N	GLN	167	31.327	33.765	31.509
	1.00	8.01						
	ATOM	1626	CA	GLN	167	30.894	33.122	30.272
10	1.00	7.76						
	ATOM	1627	CB	GLN	167	29.687	33.897	29.742
	1.00	8.57						
	ATOM	1628	CG	GLN	167	29.059	33.379	28.465
	1.00	9.03						
15	ATOM	1629	CD	GLN	167	27.822	34.189	28.116
	1.00	9.86						
	ATOM	1630	OE1	GLN	167	27.896	35.405	27.941
	1.00	9.96						
	ATOM	1631	NE2	GLN	167	26.674	33.531	28.081
20	1.00	11.48						
	ATOM	1634	C	GLN	167	32.084	33.233	29.322
	1.00	7.37						
	ATOM	1635	O	GLN	167	32.463	34.340	28.940
	1.00	7.66						
25	ATOM	1636	N	VAL	168	32.684	32.103	28.961
	1.00	6.64						
	ATOM	1638	CA	VAL	168	33.871	32.126	28.109
	1.00	6.81						
	ATOM	1639	CB	VAL	168	35.152	31.861	28.970
30	1.00	7.79						
	ATOM	1640	CG1	VAL	168	35.294	32.912	30.062
	1.00	7.77						
	ATOM	1641	CG2	VAL	168	35.093	30.475	29.599
	1.00	8.95						
35	ATOM	1642	C	VAL	168	33.857	31.097	26.992
	1.00	6.72						
	ATOM	1643	O	VAL	168	33.087	30.141	27.034
	1.00	7.62						
	ATOM	1644	N	MET	169	34.671	31.325	25.962
40	1.00	6.24						
	ATOM	1646	CA	MET	169	34.822	30.353	24.875
	1.00	7.10						
	ATOM	1647	CB	MET	169	35.078	31.020	23.527
	1.00	7.60						
45	ATOM	1648	CG	MET	169	35.016	30.028	22.389
	1.00	9.98						
	ATOM	1649	SD	MET	169	33.355	29.295	22.243
	1.00	10.60						
	ATOM	1650	CE	MET	169	33.759	27.805	21.363
50	1.00	11.26						
	ATOM	1651	C	MET	169	36.066	29.618	25.357
	1.00	7.23						
	ATOM	1652	O	MET	169	37.175	30.167	25.347
	1.00	7.62						
55	ATOM	1653	N	ALA	170	35.871	28.375	25.750
	1.00	6.93						

	ATOM	1655	CA	ALA	170	36.920	27.585	26.367
	1.00	7.05						
	ATOM	1656	CB	ALA	170	36.453	27.205	27.778
	1.00	8.93						
5	ATOM	1657	C	ALA	170	37.436	26.334	25.706
	1.00	7.41						
	ATOM	1658	O	ALA	170	36.823	25.752	24.806
	1.00	6.87						
10	ATOM	1659	N	THR	171	38.585	25.920	26.230
	1.00	7.05						
	ATOM	1661	CA	THR	171	39.218	24.668	25.892
	1.00	6.62						
	ATOM	1662	CB	THR	171	40.690	24.847	25.497
	1.00	7.70						
15	ATOM	1663	OG1	THR	171	40.771	25.554	24.258
	1.00	8.40						
	ATOM	1665	CG2	THR	171	41.363	23.476	25.341
	1.00	8.06						
20	ATOM	1666	C	THR	171	39.195	23.916	27.237
	1.00	7.48						
	ATOM	1667	O	THR	171	39.717	24.420	28.242
	1.00	7.78						
	ATOM	1668	N	GLU	172	38.507	22.778	27.290
	1.00	7.60						
25	ATOM	1670	CA	GLU	172	38.473	21.968	28.510
	1.00	7.72						
	ATOM	1671	CB	GLU	172	37.040	21.751	29.035
	1.00	8.64						
30	ATOM	1672	CG	GLU	172	37.010	20.705	30.165
	1.00	10.82						
	ATOM	1673	CD	GLU	172	35.722	20.667	30.977
	1.00	13.27						
	ATOM	1674	OE1	GLU	172	35.663	19.872	31.946
	1.00	14.50						
35	ATOM	1675	OE2	GLU	172	34.785	21.428	30.667
	1.00	13.18						
	ATOM	1676	C	GLU	172	39.085	20.613	28.180
	1.00	8.52						
40	ATOM	1677	O	GLU	172	38.843	20.069	27.101
	1.00	9.45						
	ATOM	1678	N	GLY	173	39.909	20.089	29.077
	1.00	7.84						
	ATOM	1680	CA	GLY	173	40.501	18.792	28.830
	1.00	8.42						
45	ATOM	1681	C	GLY	173	40.389	17.910	30.046
	1.00	9.01						
	ATOM	1682	O	GLY	173	40.196	18.403	31.164
	1.00	9.09						
50	ATOM	1683	N	TYR	174	40.442	16.602	29.817
	1.00	9.90						
	ATOM	1685	CA	TYR	174	40.389	15.626	30.896
	1.00	10.77						
	ATOM	1686	CB	TYR	174	38.969	15.103	31.125
	1.00	13.07						
55	ATOM	1687	CG	TYR	174	38.914	14.153	32.296
	1.00	16.61						

	ATOM	1688	CD1	TYR	174	38.603	12.811	32.115
	1.00	18.40						
	ATOM	1689	CE1	TYR	174	38.619	11.926	33.181
	1.00	19.66						
5	ATOM	1690	CD2	TYR	174	39.236	14.586	33.579
	1.00	18.49						
	ATOM	1691	CE2	TYR	174	39.258	13.709	34.648
	1.00	20.51						
10	ATOM	1692	CZ	TYR	174	38.948	12.383	34.443
	1.00	20.34						
	ATOM	1693	OH	TYR	174	38.970	11.506	35.508
	1.00	24.58						
	ATOM	1695	C	TYR	174	41.311	14.466	30.552
	1.00	10.26						
15	ATOM	1696	O	TYR	174	41.107	13.773	29.553
	1.00	10.33						
	ATOM	1697	N	GLN	175	42.359	14.308	31.359
	1.00	9.98						
	ATOM	1699	CA	GLN	175	43.354	13.248	31.184
20	1.00	10.93						
	ATOM	1700	CB	GLN	175	42.837	11.937	31.787
	1.00	13.41						
	ATOM	1701	CG	GLN	175	42.566	12.065	33.283
	1.00	16.14						
25	ATOM	1702	CD	GLN	175	42.419	10.732	34.001
	1.00	19.68						
	ATOM	1703	OE1	GLN	175	42.573	10.665	35.228
	1.00	21.27						
30	ATOM	1704	NE2	GLN	175	42.110	9.673	33.258
	1.00	20.43						
	ATOM	1707	C	GLN	175	43.781	13.073	29.720
	1.00	10.40						
	ATOM	1708	O	GLN	175	43.726	11.976	29.151
	1.00	10.98						
35	ATOM	1709	N	SER	176	44.279	14.155	29.137
	1.00	10.43						
	ATOM	1711	CA	SER	176	44.680	14.133	27.746
	1.00	9.15						
	ATOM	1712	CB	SER	176	43.467	14.513	26.879
40	1.00	10.20						
	ATOM	1713	OG	SER	176	43.042	15.847	27.130
	1.00	9.79						
	ATOM	1715	C	SER	176	45.840	15.101	27.489
	1.00	9.26						
45	ATOM	1716	O	SER	176	46.427	15.654	28.426
	1.00	9.17						
	ATOM	1717	N	SER	177	46.178	15.264	26.216
	1.00	9.64						
50	ATOM	1719	CA	SER	177	47.240	16.164	25.776
	1.00	9.15						
	ATOM	1720	CB	SER	177	48.507	15.375	25.461
	1.00	10.09						
	ATOM	1721	OG	SER	177	48.928	14.633	26.596
	1.00	12.00						
55	ATOM	1723	C	SER	177	46.745	16.829	24.508
	1.00	10.02						

	ATOM	1724	O	SER	177	45.803	16.341	23.883
	1.00	9.82						
	ATOM	1725	N	GLY	178	47.317	17.972	24.157
	1.00	9.77						
5	ATOM	1727	CA	GLY	178	46.893	18.632	22.935
	1.00	9.38						
	ATOM	1728	C	GLY	178	47.289	20.089	22.869
	1.00	9.30						
10	ATOM	1729	O	GLY	178	48.044	20.569	23.714
	1.00	8.99						
	ATOM	1730	N	SER	179	46.757	20.785	21.870
	1.00	9.17						
	ATOM	1732	CA	SER	179	47.028	22.206	21.674
	1.00	9.44						
15	ATOM	1733	CB	SER	179	48.177	22.408	20.671
	1.00	11.55						
	ATOM	1734	OG	SER	179	49.424	22.073	21.243
	1.00	19.58						
	ATOM	1736	C	SER	179	45.804	22.901	21.104
20	1.00	8.63						
	ATOM	1737	O	SER	179	45.009	22.284	20.394
	1.00	9.53						
	ATOM	1738	N	SER	180	45.636	24.164	21.463
	1.00	8.95						
25	ATOM	1740	CA	SER	180	44.563	24.989	20.937
	1.00	8.51						
	ATOM	1741	CB	SER	180	43.263	24.866	21.750
	1.00	9.65						
	ATOM	1742	OG	SER	180	43.365	25.508	23.006
30	1.00	11.87						
	ATOM	1744	C	SER	180	45.026	26.441	20.912
	1.00	8.80						
	ATOM	1745	O	SER	180	45.920	26.848	21.674
	1.00	9.51						
35	ATOM	1746	N	ASN	181	44.454	27.202	19.993
	1.00	8.43						
	ATOM	1748	CA	ASN	181	44.750	28.619	19.850
	1.00	8.44						
	ATOM	1749	CB	ASN	181	45.837	28.845	18.792
40	1.00	9.20						
	ATOM	1750	CG	ASN	181	46.374	30.257	18.808
	1.00	10.45						
	ATOM	1751	OD1	ASN	181	47.577	30.476	19.001
	1.00	14.84						
45	ATOM	1752	ND2	ASN	181	45.504	31.221	18.607
	1.00	9.73						
	ATOM	1755	C	ASN	181	43.406	29.157	19.385
	1.00	8.65						
	ATOM	1756	O	ASN	181	42.912	28.774	18.322
50	1.00	8.58						
	ATOM	1757	N	VAL	182	42.802	30.003	20.211
	1.00	7.83						
	ATOM	1759	CA	VAL	182	41.474	30.535	19.940
	1.00	7.20						
55	ATOM	1760	CB	VAL	182	40.449	29.879	20.899
	1.00	8.34						

	ATOM	1761	CG1	VAL	182	39.018	30.269	20.525
	1.00	9.23						
	ATOM	1762	CG2	VAL	182	40.612	28.362	20.910
	1.00	8.07						
5	ATOM	1763	C	VAL	182	41.411	32.046	20.158
	1.00	8.01						
	ATOM	1764	O	VAL	182	42.013	32.576	21.097
	1.00	7.62						
	ATOM	1765	N	THR	183	40.646	32.728	19.311
10	1.00	7.00						
	ATOM	1767	CA	THR	183	40.459	34.173	19.418
	1.00	7.39						
	ATOM	1768	CB	THR	183	40.973	34.877	18.146
	1.00	8.24						
15	ATOM	1769	OG1	THR	183	42.362	34.565	17.995
	1.00	9.42						
	ATOM	1771	CG2	THR	183	40.799	36.398	18.245
	1.00	8.99						
	ATOM	1772	C	THR	183	38.964	34.373	19.603
20	1.00	7.65						
	ATOM	1773	O	THR	183	38.166	33.828	18.834
	1.00	7.43						
	ATOM	1774	N	VAL	184	38.595	35.121	20.634
	1.00	7.62						
25	ATOM	1776	CA	VAL	184	37.194	35.351	20.999
	1.00	8.26						
	ATOM	1777	CB	VAL	184	36.979	34.886	22.464
	1.00	9.19						
	ATOM	1778	CG1	VAL	184	35.502	34.914	22.837
30	1.00	9.70						
	ATOM	1779	CG2	VAL	184	37.576	33.502	22.672
	1.00	9.78						
	ATOM	1780	C	VAL	184	36.829	36.832	20.938
	1.00	8.76						
35	ATOM	1781	O	VAL	184	37.637	37.674	21.330
	1.00	8.92						
	ATOM	1782	N	TRP	185	35.619	37.144	20.461
	1.00	8.50						
	ATOM	1784	CA	TRP	185	35.142	38.525	20.401
40	1.00	9.38						
	ATOM	1785	CB	TRP	185	35.755	39.295	19.212
	1.00	9.55						
	ATOM	1786	CG	TRP	185	35.302	38.875	17.840
	1.00	10.25						
45	ATOM	1787	CD2	TRP	185	35.814	37.791	17.055
	1.00	10.55						
	ATOM	1788	CE2	TRP	185	35.150	37.825	15.808
	1.00	10.75						
	ATOM	1789	CE3	TRP	185	36.769	36.797	17.281
50	1.00	10.39						
	ATOM	1790	CD1	TRP	185	34.367	39.497	17.061
	1.00	11.62						
	ATOM	1791	NE1	TRP	185	34.272	38.876	15.840
	1.00	12.03						
55	ATOM	1793	CZ2	TRP	185	35.410	36.903	14.794
	1.00	11.32						

	ATOM	1794	CZ3	TRP	185	37.025	35.883	16.266
	1.00	11.87						
	ATOM	1795	CH2	TRP	185	36.346	35.944	15.040
	1.00	11.03						
5	ATOM	1796	C	TRP	185	33.611	38.581	20.364
	1.00	9.55						
	ATOM	1797	O	TRP	185	32.974	37.509	20.372
	1.00	9.75						
10	ATOM	1798	OXT	TRP	185	33.062	39.698	20.362
	1.00	12.79						

The three-dimensional crystal structure of the *T. harzianum* xylanase shows a great degree of similarity to the structure of the *B. circulans* xylanase (Figure 3), although the *T. harzianum* xylanase contains two extra strands at the beginning of sheets I and II, and a few small insertions and deletions (see also Figure 1). While the structures are similar at 89% of the residues of the *B. circulans* xylanase, the sequences are identical at only 51% of the 185 residues. The x-ray co-ordinates of the structure is given below.

	ATOM	1	CB	GLN	1	15.828	12.804	3.943
	1.00	26.76						
25	ATOM	2	CG	GLN	1	14.520	12.576	3.185
	1.00	31.36						
	ATOM	3	CD	GLN	1	13.427	13.621	3.366
	1.00	32.78						
30	ATOM	4	OE1	GLN	1	13.524	14.505	4.210
	1.00	35.55						
	ATOM	5	NE2	GLN	1	12.296	13.583	2.708
	1.00	35.11						
	ATOM	6	C	GLN	1	17.269	13.179	5.908
	1.00	24.81						
35	ATOM	7	O	GLN	1	18.126	13.319	5.064
	1.00	27.64						
	ATOM	8	N	GLN	1	15.208	13.707	6.190
	1.00	24.75						
40	ATOM	9	CA	GLN	1	15.926	12.688	5.486
	1.00	25.70						
	ATOM	10	N	THR	2	17.472	13.314	7.213
	1.00	25.76						
	ATOM	11	CA	THR	2	18.554	14.044	7.875
	1.00	24.44						
45	ATOM	12	CB	THR	2	19.855	13.864	7.084
	1.00	25.32						
	ATOM	13	OG1	THR	2	20.017	12.431	7.146
	1.00	26.72						

	ATOM	14	CG2	THR	2	21.104	14.549	7.600
	1.00	27.32						
	ATOM	15	C	THR	2	17.847	15.388	7.733
	1.00	21.71						
5	ATOM	16	O	THR	2	17.768	16.039	6.692
	1.00	20.85						
	ATOM	17	N	ILE	3	17.002	15.542	8.751
	1.00	18.32						
	ATOM	18	CA	ILE	3	16.196	16.735	8.873
10	1.00	17.14						
	ATOM	19	CB	ILE	3	14.723	16.216	8.640
	1.00	17.94						
	ATOM	20	CG2	ILE	3	13.680	16.289	9.744
	1.00	16.71						
15	ATOM	21	CG1	ILE	3	14.269	17.095	7.557
	1.00	18.00						
	ATOM	22	CD1	ILE	3	14.803	16.716	6.179
	1.00	20.15						
	ATOM	23	C	ILE	3	16.568	17.281	10.229
20	1.00	16.13						
	ATOM	24	O	ILE	3	17.085	16.584	11.119
	1.00	16.34						
	ATOM	25	N	GLY	4	16.451	18.588	10.370
	1.00	14.88						
25	ATOM	26	CA	GLY	4	16.674	19.198	11.659
	1.00	11.55						
	ATOM	27	C	GLY	4	15.299	19.349	12.251
	1.00	12.16						
	ATOM	28	O	GLY	4	14.314	18.938	11.628
30	1.00	11.77						
	ATOM	29	N	PRO	5	15.134	19.926	13.445
	1.00	11.94						
	ATOM	30	CD	PRO	5	16.159	20.593	14.231
	1.00	12.27						
35	ATOM	31	CA	PRO	5	13.887	19.803	14.160
	1.00	12.67						
	ATOM	32	CB	PRO	5	14.208	20.405	15.490
	1.00	12.77						
	ATOM	33	CG	PRO	5	15.703	20.207	15.627
40	1.00	12.89						
	ATOM	34	C	PRO	5	12.754	20.463	13.391
	1.00	13.39						
	ATOM	35	O	PRO	5	12.974	21.493	12.764
	1.00	14.17						
45	ATOM	36	N	GLY	6	11.583	19.867	13.377
	1.00	12.31						
	ATOM	37	CA	GLY	6	10.494	20.387	12.606
	1.00	13.71						
	ATOM	38	C	GLY	6	9.260	19.487	12.636
50	1.00	14.99						
	ATOM	39	O	GLY	6	9.172	18.391	13.233
	1.00	14.55						
	ATOM	40	N	THR	7	8.292	19.986	11.875
	1.00	15.50						
55	ATOM	41	CA	THR	7	6.963	19.390	11.753
	1.00	15.99						

	ATOM	42	CB	THR	7	6.093	20.345	12.625
	1.00	16.25						
	ATOM	43	OG1	THR	7	5.671	19.625	13.799
	1.00	16.71						
5	ATOM	44	CG2	THR	7	4.986	20.941	11.844
	1.00	16.56						
	ATOM	45	C	THR	7	6.671	19.383	10.249
	1.00	17.13						
10	ATOM	46	O	THR	7	7.171	20.278	9.526
	1.00	16.03						
	ATOM	47	N	GLY	8	5.941	18.369	9.742
	1.00	18.40						
	ATOM	48	CA	GLY	8	5.511	18.374	8.345
	1.00	19.41						
15	ATOM	49	C	GLY	8	4.948	17.020	7.930
	1.00	20.80						
	ATOM	50	O	GLY	8	4.664	16.135	8.751
	1.00	20.52						
20	ATOM	51	N	TYR	9	4.868	16.856	6.621
	1.00	23.10						
	ATOM	52	CA	TYR	9	4.319	15.669	5.985
	1.00	24.71						
	ATOM	53	CB	TYR	9	3.106	15.980	5.152
	1.00	23.68						
25	ATOM	54	CG	TYR	9	1.919	16.159	6.053
	1.00	23.21						
	ATOM	55	CD1	TYR	9	1.098	15.072	6.302
	1.00	24.08						
30	ATOM	56	CE1	TYR	9	0.066	15.221	7.201
	1.00	24.07						
	ATOM	57	CD2	TYR	9	1.719	17.380	6.663
	1.00	23.62						
	ATOM	58	CE2	TYR	9	0.686	17.525	7.566
	1.00	24.15						
35	ATOM	59	CZ	TYR	9	-0.118	16.437	7.827
	1.00	23.90						
	ATOM	60	OH	TYR	9	-1.099	16.569	8.790
	1.00	24.93						
40	ATOM	61	C	TYR	9	5.307	15.026	5.047
	1.00	26.87						
	ATOM	62	O	TYR	9	6.094	15.819	4.503
	1.00	26.77						
	ATOM	63	N	SER	10	5.354	13.666	4.903
	1.00	29.24						
45	ATOM	64	CA	SER	10	6.074	13.019	3.786
	1.00	31.30						
	ATOM	65	CB	SER	10	7.578	12.994	4.132
	1.00	33.29						
50	ATOM	66	OG	SER	10	8.099	14.175	3.415
	1.00	36.05						
	ATOM	67	C	SER	10	5.687	11.658	3.167
	1.00	31.30						
	ATOM	68	O	SER	10	6.443	10.761	2.742
	1.00	32.28						
55	ATOM	69	N	ASN	11	4.369	11.565	3.067
	1.00	31.13						

	ATOM	70	CA	ASN	11	3.633	10.727	2.104
	1.00	29.54						
	ATOM	71	CB	ASN	11	4.369	9.574	1.411
	1.00	31.69						
5	ATOM	72	CG	ASN	11	3.862	9.653	-0.044
	1.00	34.14						
	ATOM	73	OD1	ASN	11	2.642	9.754	-0.339
	1.00	33.69						
	ATOM	74	ND2	ASN	11	4.801	9.795	-0.993
10	1.00	34.10						
	ATOM	75	C	ASN	11	2.473	10.070	2.756
	1.00	27.90						
	ATOM	76	O	ASN	11	2.349	8.838	2.987
	1.00	28.07						
15	ATOM	77	N	GLY	12	1.757	11.137	3.151
	1.00	24.30						
	ATOM	78	CA	GLY	12	0.547	10.965	3.909
	1.00	22.09						
	ATOM	79	C	GLY	12	0.839	10.928	5.400
20	1.00	19.23						
	ATOM	80	O	GLY	12	-0.117	10.901	6.189
	1.00	19.87						
	ATOM	81	N	TYR	13	2.112	10.925	5.828
	1.00	16.68						
25	ATOM	82	CA	TYR	13	2.364	10.901	7.256
	1.00	13.96						
	ATOM	83	CB	TYR	13	3.311	9.730	7.672
	1.00	14.86						
	ATOM	84	CG	TYR	13	2.641	8.380	7.359
30	1.00	16.63						
	ATOM	85	CD1	TYR	13	1.913	7.701	8.331
	1.00	18.73						
	ATOM	86	CE1	TYR	13	1.274	6.499	7.999
	1.00	19.94						
35	ATOM	87	CD2	TYR	13	2.730	7.866	6.084
	1.00	16.53						
	ATOM	88	CE2	TYR	13	2.101	6.680	5.740
	1.00	17.13						
	ATOM	89	CZ	TYR	13	1.384	6.020	6.710
40	1.00	18.35						
	ATOM	90	OH	TYR	13	0.758	4.855	6.377
	1.00	19.27						
	ATOM	91	C	TYR	13	2.988	12.206	7.686
	1.00	12.85						
45	ATOM	92	O	TYR	13	3.768	12.869	7.013
	1.00	11.47						
	ATOM	93	N	TYR	14	2.469	12.560	8.828
	1.00	14.13						
	ATOM	94	CA	TYR	14	2.901	13.680	9.583
50	1.00	12.57						
	ATOM	95	CB	TYR	14	1.785	13.965	10.526
	1.00	13.51						
	ATOM	96	CG	TYR	14	2.119	15.111	11.446
	1.00	15.53						
55	ATOM	97	CD1	TYR	14	2.055	16.416	10.949
	1.00	16.07						

	ATOM	98	CE1	TYR	14	2.374	17.464	11.785
	1.00	15.89						
	ATOM	99	CD2	TYR	14	2.497	14.849	12.762
	1.00	16.13						
5	ATOM	100	CE2	TYR	14	2.827	15.898	13.594
	1.00	16.08						
	ATOM	101	CZ	TYR	14	2.748	17.186	13.077
	1.00	16.73						
10	ATOM	102	OH	TYR	14	3.055	18.266	13.866
	1.00	18.42						
	ATOM	103	C	TYR	14	4.165	13.171	10.274
	1.00	13.04						
	ATOM	104	O	TYR	14	4.290	11.986	10.656
	1.00	11.98						
15	ATOM	105	N	TYR	15	5.107	14.068	10.452
	1.00	11.94						
	ATOM	106	CA	TYR	15	6.302	13.775	11.193
	1.00	12.73						
20	ATOM	107	CB	TYR	15	7.551	13.590	10.265
	1.00	15.06						
	ATOM	108	CG	TYR	15	8.113	14.812	9.520
	1.00	17.13						
	ATOM	109	CD1	TYR	15	7.729	15.025	8.221
	1.00	17.27						
25	ATOM	110	CE1	TYR	15	8.165	16.146	7.558
	1.00	18.57						
	ATOM	111	CD2	TYR	15	8.954	15.714	10.164
	1.00	18.44						
30	ATOM	112	CE2	TYR	15	9.389	16.845	9.506
	1.00	18.53						
	ATOM	113	CZ	TYR	15	8.983	17.056	8.207
	1.00	19.40						
	ATOM	114	OH	TYR	15	9.324	18.241	7.554
	1.00	21.86						
35	ATOM	115	C	TYR	15	6.470	14.984	12.096
	1.00	12.96						
	ATOM	116	O	TYR	15	6.048	16.114	11.732
	1.00	10.33						
40	ATOM	117	N	SER	16	7.095	14.681	13.245
	1.00	11.29						
	ATOM	118	CA	SER	16	7.450	15.700	14.199
	1.00	11.41						
	ATOM	119	CB	SER	16	6.416	15.772	15.316
	1.00	9.89						
45	ATOM	120	OG	SER	16	6.764	16.764	16.281
	1.00	10.30						
	ATOM	121	C	SER	16	8.790	15.268	14.773
	1.00	12.00						
50	ATOM	122	O	SER	16	8.944	14.112	15.217
	1.00	13.12						
	ATOM	123	N	TYR	17	9.787	16.126	14.795
	1.00	10.82						
	ATOM	124	CA	TYR	17	11.047	15.823	15.405
	1.00	8.67						
55	ATOM	125	CB	TYR	17	12.079	15.633	14.307
	1.00	7.15						



	ATOM	126	CG	TYR	17	13.533	15.647	14.771
	1.00	7.03						
	ATOM	127	CD1	TYR	17	13.886	15.191	16.039
	1.00	7.12						
5	ATOM	128	CE1	TYR	17	15.186	15.210	16.456
	1.00	7.12						
	ATOM	129	CD2	TYR	17	14.502	16.123	13.920
	1.00	6.69						
	ATOM	130	CE2	TYR	17	15.808	16.140	14.325
10	1.00	7.74						
	ATOM	131	CZ	TYR	17	16.131	15.685	15.596
	1.00	7.93						
	ATOM	132	OH	TYR	17	17.422	15.747	16.038
	1.00	7.83						
15	ATOM	133	C	TYR	17	11.329	17.058	16.262
	1.00	10.23						
	ATOM	134	O	TYR	17	11.442	18.156	15.702
	1.00	11.78						
	ATOM	135	N	TRP	18	11.511	16.898	17.564
20	1.00	11.36						
	ATOM	136	CA	TRP	18	11.782	17.983	18.516
	1.00	13.34						
	ATOM	137	CB	TRP	18	10.624	18.138	19.571
	1.00	13.58						
25	ATOM	138	CG	TRP	18	11.022	19.043	20.770
	1.00	16.90						
	ATOM	139	CD2	TRP	18	11.668	18.676	21.973
	1.00	15.25						
	ATOM	140	CE2	TRP	18	11.923	19.930	22.560
30	1.00	14.76						
	ATOM	141	CE3	TRP	18	12.079	17.518	22.620
	1.00	14.38						
	ATOM	142	CD1	TRP	18	10.884	20.432	20.676
	1.00	15.60						
35	ATOM	143	NE1	TRP	18	11.444	20.923	21.780
	1.00	15.81						
	ATOM	144	CZ2	TRP	18	12.581	20.047	23.752
	1.00	12.46						
	ATOM	145	CZ3	TRP	18	12.739	17.626	23.821
40	1.00	14.47						
	ATOM	146	CH2	TRP	18	12.988	18.880	24.379
	1.00	15.27						
	ATOM	147	C	TRP	18	13.076	17.609	19.261
	1.00	14.41						
45	ATOM	148	O	TRP	18	13.287	16.436	19.642
	1.00	13.85						
	ATOM	149	N	ASN	19	13.984	18.545	19.526
	1.00	12.84						
	ATOM	150	CA	ASN	19	15.035	18.250	20.451
50	1.00	13.21						
	ATOM	151	CB	ASN	19	16.224	17.600	19.699
	1.00	14.57						
	ATOM	152	CG	ASN	19	17.151	18.440	18.894
	1.00	15.06						
55	ATOM	153	OD1	ASN	19	17.244	19.629	19.124
	1.00	18.68						



	ATOM	154	ND2	ASN	19	17.864	17.941	17.903
	1.00	16.80						
	ATOM	155	C	ASN	19	15.396	19.550	21.166
	1.00	12.55						
5	ATOM	156	O	ASN	19	14.989	20.636	20.741
	1.00	13.22						
	ATOM	157	N	ASP	20	16.131	19.441	22.251
	1.00	11.88						
10	ATOM	158	CA	ASP	20	16.504	20.540	23.135
	1.00	11.46						
	ATOM	159	CB	ASP	20	16.797	19.893	24.518
	1.00	10.44						
	ATOM	160	CG	ASP	20	18.025	18.968	24.621
	1.00	9.88						
15	ATOM	161	OD1	ASP	20	18.718	18.720	23.650
	1.00	10.13						
	ATOM	162	OD2	ASP	20	18.310	18.428	25.678
	1.00	10.16						
20	ATOM	163	C	ASP	20	17.695	21.403	22.637
	1.00	11.25						
	ATOM	164	O	ASP	20	18.103	22.388	23.291
	1.00	13.63						
	ATOM	165	N	GLY	21	18.234	21.045	21.466
	1.00	9.37						
25	ATOM	166	CA	GLY	21	19.380	21.652	20.875
	1.00	8.25						
	ATOM	167	C	GLY	21	20.648	20.856	21.103
	1.00	9.30						
30	ATOM	168	O	GLY	21	21.648	21.119	20.438
	1.00	8.94						
	ATOM	169	N	HIS	22	20.741	19.936	22.053
	1.00	9.49						
	ATOM	170	CA	HIS	22	21.960	19.155	22.258
	1.00	8.32						
35	ATOM	171	CB	HIS	22	21.741	18.177	23.358
	1.00	8.11						
	ATOM	172	CG	HIS	22	22.979	17.601	23.957
	1.00	6.81						
40	ATOM	173	CD2	HIS	22	23.428	18.016	25.187
	1.00	6.67						
	ATOM	174	ND1	HIS	22	23.803	16.685	23.489
	1.00	8.56						
	ATOM	175	CE1	HIS	22	24.747	16.526	24.386
	1.00	8.59						
45	ATOM	176	NE2	HIS	22	24.505	17.334	25.395
	1.00	8.33						
	ATOM	177	C	HIS	22	22.310	18.377	20.984
	1.00	8.28						
50	ATOM	178	O	HIS	22	21.423	17.986	20.218
	1.00	9.57						
	ATOM	179	N	ALA	23	23.598	18.178	20.750
	1.00	6.80						
	ATOM	180	CA	ALA	23	24.077	17.456	19.601
	1.00	8.20						
55	ATOM	181	CB	ALA	23	25.543	17.722	19.414
	1.00	6.23						

	ATOM	182	C	ALA	23	23.884	15.951	19.853
	1.00	9.20						
	ATOM	183	O	ALA	23	23.555	15.546	20.983
	1.00	9.54						
5	ATOM	184	N	GLY	24	24.053	15.132	18.813
	1.00	11.67						
	ATOM	185	CA	GLY	24	24.056	13.696	19.026
	1.00	11.28						
	ATOM	186	C	GLY	24	23.003	12.932	18.274
10	1.00	12.70						
	ATOM	187	O	GLY	24	23.144	11.705	18.119
	1.00	14.05						
	ATOM	188	N	VAL	25	21.954	13.601	17.782
	1.00	11.17						
15	ATOM	189	CA	VAL	25	20.870	12.933	17.087
	1.00	11.42						
	ATOM	190	CB	VAL	25	19.513	13.475	17.632
	1.00	10.39						
	ATOM	191	CG1	VAL	25	18.430	12.519	17.220
20	1.00	9.36						
	ATOM	192	CG2	VAL	25	19.568	13.692	19.147
	1.00	10.78						
	ATOM	193	C	VAL	25	20.893	13.113	15.566
	1.00	11.41						
25	ATOM	194	O	VAL	25	21.215	14.214	15.055
	1.00	10.88						
	ATOM	195	N	THR	26	20.545	12.071	14.797
	1.00	12.50						
	ATOM	196	CA	THR	26	20.256	12.290	13.397
30	1.00	12.14						
	ATOM	197	CB	THR	26	21.498	11.864	12.462
	1.00	13.95						
	ATOM	198	OG1	THR	26	21.030	10.946	11.485
	1.00	16.06						
35	ATOM	199	CG2	THR	26	22.706	11.411	13.230
	1.00	12.20						
	ATOM	200	C	THR	26	18.959	11.552	13.126
	1.00	12.76						
	ATOM	201	O	THR	26	18.758	10.385	13.519
40	1.00	13.16						
	ATOM	202	N	TYR	27	17.998	12.359	12.665
	1.00	10.77						
	ATOM	203	CA	TYR	27	16.665	11.919	12.311
	1.00	10.37						
45	ATOM	204	CB	TYR	27	15.581	12.842	12.861
	1.00	9.29						
	ATOM	205	CG	TYR	27	14.148	12.477	12.477
	1.00	8.75						
	ATOM	206	CD1	TYR	27	13.599	12.815	11.240
50	1.00	9.08						
	ATOM	207	CE1	TYR	27	12.306	12.458	10.929
	1.00	10.58						
	ATOM	208	CD2	TYR	27	13.378	11.789	13.377
	1.00	8.03						
55	ATOM	209	CE2	TYR	27	12.077	11.427	13.078
	1.00	8.62						

	ATOM	210	CZ	TYR	27	11.547	11.760	11.854
	1.00	10.33						
	ATOM	211	OH	TYR	27	10.269	11.337	11.544
	1.00	11.41						
5	ATOM	212	C	TYR	27	16.526	11.902	10.789
	1.00	10.52						
	ATOM	213	O	TYR	27	16.581	12.905	10.043
	1.00	9.97						
10	ATOM	214	N	THR	28	16.226	10.719	10.289
	1.00	10.67						
	ATOM	215	CA	THR	28	15.990	10.624	8.866
	1.00	13.02						
	ATOM	216	CB	THR	28	17.060	9.679	8.276
	1.00	12.93						
15	ATOM	217	OG1	THR	28	18.323	10.097	8.775
	1.00	14.75						
	ATOM	218	CG2	THR	28	17.051	9.700	6.740
	1.00	12.92						
20	ATOM	219	C	THR	28	14.577	10.154	8.537
	1.00	13.28						
	ATOM	220	O	THR	28	14.095	9.159	9.058
	1.00	11.76						
	ATOM	221	N	ASN	29	13.877	10.924	7.712
	1.00	15.11						
25	ATOM	222	CA	ASN	29	12.610	10.493	7.127
	1.00	17.11						
	ATOM	223	CB	ASN	29	11.759	11.680	6.583
	1.00	20.17						
30	ATOM	224	CG	ASN	29	10.957	11.330	5.310
	1.00	23.95						
	ATOM	225	OD1	ASN	29	9.752	11.006	5.349
	1.00	25.19						
	ATOM	226	ND2	ASN	29	11.595	11.263	4.123
	1.00	26.04						
35	ATOM	227	C	ASN	29	12.949	9.585	5.931
	1.00	17.45						
	ATOM	228	O	ASN	29	13.733	9.976	5.034
	1.00	13.40						
40	ATOM	229	N	GLY	30	12.292	8.430	5.973
	1.00	17.19						
	ATOM	230	CA	GLY	30	12.366	7.507	4.876
	1.00	20.59						
	ATOM	231	C	GLY	30	11.061	7.603	4.091
	1.00	20.60						
45	ATOM	232	O	GLY	30	10.149	8.393	4.394
	1.00	21.82						
	ATOM	233	N	GLY	31	10.880	6.783	3.065
	1.00	20.69						
50	ATOM	234	CA	GLY	31	9.593	6.864	2.353
	1.00	21.04						
	ATOM	235	C	GLY	31	8.379	6.433	3.198
	1.00	20.17						
	ATOM	236	O	GLY	31	8.534	5.626	4.140
	1.00	21.45						
55	ATOM	237	N	GLY	32	7.192	7.004	2.901
	1.00	17.60						

	ATOM	238	CA	GLY	32	5.921	6.633	3.522
	1.00	15.29						
	ATOM	239	C	GLY	32	5.950	6.688	5.053
	1.00	13.27						
5	ATOM	240	O	GLY	32	6.228	7.744	5.678
	1.00	14.99						
	ATOM	241	N	GLY	33	5.743	5.536	5.682
	1.00	10.93						
10	ATOM	242	CA	GLY	33	5.684	5.504	7.127
	1.00	9.50						
	ATOM	243	C	GLY	33	7.020	5.351	7.849
	1.00	7.59						
	ATOM	244	O	GLY	33	7.024	5.171	9.070
	1.00	6.40						
15	ATOM	245	N	SER	34	8.144	5.399	7.165
	1.00	7.69						
	ATOM	246	CA	SER	34	9.433	5.095	7.768
	1.00	9.77						
20	ATOM	247	CB	SER	34	10.348	4.331	6.832
	1.00	9.92						
	ATOM	248	OG	SER	34	9.840	3.098	6.383
	1.00	11.79						
	ATOM	249	C	SER	34	10.278	6.253	8.213
	1.00	8.85						
25	ATOM	250	O	SER	34	10.312	7.296	7.519
	1.00	11.44						
	ATOM	251	N	PHE	35	10.938	6.029	9.340
	1.00	8.14						
30	ATOM	252	CA	PHE	35	11.958	6.938	9.798
	1.00	7.22						
	ATOM	253	CB	PHE	35	11.353	8.045	10.667
	1.00	5.37						
	ATOM	254	CG	PHE	35	10.780	7.622	11.990
	1.00	4.40						
35	ATOM	255	CD1	PHE	35	9.482	7.189	12.055
	1.00	5.29						
	ATOM	256	CD2	PHE	35	11.578	7.664	13.111
	1.00	2.70						
40	ATOM	257	CE1	PHE	35	8.972	6.789	13.273
	1.00	5.43						
	ATOM	258	CE2	PHE	35	11.073	7.267	14.314
	1.00	4.23						
	ATOM	259	CZ	PHE	35	9.772	6.828	14.399
	1.00	5.42						
45	ATOM	260	C	PHE	35	12.974	6.128	10.596
	1.00	7.01						
	ATOM	261	O	PHE	35	12.624	5.078	11.148
	1.00	7.90						
50	ATOM	262	N	THR	36	14.193	6.657	10.651
	1.00	6.93						
	ATOM	263	CA	THR	36	15.346	6.181	11.379
	1.00	8.26						
	ATOM	264	CB	THR	36	16.530	5.882	10.407
	1.00	9.23						
55	ATOM	265	OG1	THR	36	15.996	5.076	9.379
	1.00	10.78						

	ATOM	266	CG2	THR	36	17.701	5.125	11.030
	1.00	10.22						
	ATOM	267	C	THR	36	15.758	7.312	12.343
	1.00	9.84						
5	ATOM	268	O	THR	36	15.537	8.507	12.050
	1.00	9.61						
	ATOM	269	N	VAL	37	16.298	6.977	13.520
	1.00	9.80						
10	ATOM	270	CA	VAL	37	16.826	7.961	14.439
	1.00	9.70						
	ATOM	271	CB	VAL	37	15.976	8.312	15.692
	1.00	10.77						
	ATOM	272	CG1	VAL	37	16.624	9.555	16.323
	1.00	10.77						
15	ATOM	273	CG2	VAL	37	14.509	8.571	15.389
	1.00	10.75						
	ATOM	274	C	VAL	37	18.010	7.180	14.958
	1.00	10.19						
20	ATOM	275	O	VAL	37	17.903	5.987	15.292
	1.00	12.44						
	ATOM	276	N	ASN	38	19.154	7.842	15.003
	1.00	9.51						
	ATOM	277	CA	ASN	38	20.363	7.273	15.517
	1.00	10.83						
25	ATOM	278	CB	ASN	38	21.351	7.007	14.392
	1.00	13.08						
	ATOM	279	CG	ASN	38	20.884	5.745	13.683
	1.00	18.12						
30	ATOM	280	OD1	ASN	38	20.079	5.762	12.722
	1.00	18.42						
	ATOM	281	ND2	ASN	38	21.365	4.580	14.159
	1.00	18.73						
	ATOM	282	C	ASN	38	20.878	8.342	16.455
	1.00	10.89						
35	ATOM	283	O	ASN	38	20.817	9.510	16.083
	1.00	10.36						
	ATOM	284	N	TRP	39	21.339	8.018	17.651
	1.00	8.76						
40	ATOM	285	CA	TRP	39	21.772	9.048	18.577
	1.00	10.30						
	ATOM	286	CB	TRP	39	20.583	9.478	19.449
	1.00	8.23						
	ATOM	287	CG	TRP	39	19.943	8.426	20.359
	1.00	7.73						
45	ATOM	288	CD2	TRP	39	19.034	7.452	19.994
	1.00	7.65						
	ATOM	289	CE2	TRP	39	18.728	6.903	21.234
	1.00	7.27						
50	ATOM	290	CE3	TRP	39	18.410	6.956	18.835
	1.00	8.18						
	ATOM	291	CD1	TRP	39	20.183	8.466	21.706
	1.00	5.84						
	ATOM	292	NE1	TRP	39	19.425	7.538	22.200
	1.00	5.45						
55	ATOM	293	CZ2	TRP	39	17.805	5.847	21.320
	1.00	6.19						

	ATOM	294	CZ3	TRP	39	17.487	5.910	18.934
	1.00	6.98						
	ATOM	295	CH2	TRP	39	17.194	5.367	20.174
	1.00	6.37						
5	ATOM	296	C	TRP	39	22.898	8.504	19.411
	1.00	10.96						
	ATOM	297	O	TRP	39	22.879	7.317	19.771
	1.00	13.55						
10	ATOM	298	N	SER	40	23.916	9.328	19.631
	1.00	13.07						
	ATOM	299	CA	SER	40	25.061	9.010	20.463
	1.00	13.74						
	ATOM	300	CB	SER	40	26.357	8.815	19.658
	1.00	14.37						
15	ATOM	301	OG	SER	40	26.111	7.978	18.518
	1.00	20.42						
	ATOM	302	C	SER	40	25.227	10.244	21.326
	1.00	12.72						
20	ATOM	303	O	SER	40	25.357	11.332	20.770
	1.00	10.52						
	ATOM	304	N	ASN	41	25.165	10.040	22.646
	1.00	13.35						
	ATOM	305	CA	ASN	41	25.338	11.092	23.656
	1.00	13.53						
25	ATOM	306	CB	ASN	41	26.757	11.568	23.695
	1.00	15.67						
	ATOM	307	CG	ASN	41	27.771	10.495	24.008
	1.00	18.65						
30	ATOM	308	OD1	ASN	41	28.757	10.358	23.282
	1.00	22.59						
	ATOM	309	ND2	ASN	41	27.653	9.675	25.050
	1.00	19.49						
	ATOM	310	C	ASN	41	24.441	12.287	23.350
	1.00	12.66						
35	ATOM	311	O	ASN	41	24.873	13.422	23.078
	1.00	11.83						
	ATOM	312	N	SER	42	23.155	11.974	23.365
	1.00	10.43						
40	ATOM	313	CA	SER	42	22.156	12.925	22.935
	1.00	10.63						
	ATOM	314	CB	SER	42	20.894	12.124	22.555
	1.00	9.58						
	ATOM	315	OG	SER	42	20.288	11.609	23.751
	1.00	8.86						
45	ATOM	316	C	SER	42	21.856	13.905	24.087
	1.00	9.67						
	ATOM	317	O	SER	42	22.501	13.874	25.146
	1.00	11.35						
50	ATOM	318	N	GLY	43	20.855	14.769	23.867
	1.00	9.05						
	ATOM	319	CA	GLY	43	20.215	15.460	24.946
	1.00	6.67						
	ATOM	320	C	GLY	43	18.840	14.815	25.018
	1.00	7.83						
55	ATOM	321	O	GLY	43	18.694	13.583	24.897
	1.00	9.11						

	ATOM	322	N	ASN	44	17.809	15.616	25.181
	1.00	6.80						
	ATOM	323	CA	ASN	44	16.450	15.160	25.134
	1.00	8.62						
5	ATOM	324	CB	ASN	44	15.643	15.843	26.251
	1.00	9.32						
	ATOM	325	CG	ASN	44	14.239	15.305	26.407
	1.00	11.76						
10	ATOM	326	OD1	ASN	44	13.395	16.034	26.942
	1.00	14.29						
	ATOM	327	ND2	ASN	44	13.867	14.062	26.021
	1.00	12.06						
	ATOM	328	C	ASN	44	15.906	15.528	23.737
	1.00	8.95						
15	ATOM	329	O	ASN	44	16.070	16.664	23.240
	1.00	7.76						
	ATOM	330	N	PHE	45	15.358	14.499	23.068
	1.00	8.42						
	ATOM	331	CA	PHE	45	14.723	14.592	21.745
20	1.00	8.92						
	ATOM	332	CB	PHE	45	15.707	14.187	20.598
	1.00	6.83						
	ATOM	333	CG	PHE	45	16.041	12.710	20.589
	1.00	7.80						
25	ATOM	334	CD1	PHE	45	15.274	11.836	19.819
	1.00	7.09						
	ATOM	335	CD2	PHE	45	17.051	12.228	21.403
	1.00	7.62						
	ATOM	336	CE1	PHE	45	15.515	10.477	19.875
30	1.00	7.59						
	ATOM	337	CE2	PHE	45	17.274	10.857	21.433
	1.00	7.17						
	ATOM	338	CZ	PHE	45	16.510	9.994	20.678
	1.00	5.89						
35	ATOM	339	C	PHE	45	13.491	13.660	21.684
	1.00	8.27						
	ATOM	340	O	PHE	45	13.435	12.692	22.478
	1.00	9.67						
	ATOM	341	N	VAL	46	12.541	13.912	20.755
40	1.00	7.23						
	ATOM	342	CA	VAL	46	11.346	13.130	20.533
	1.00	7.92						
	ATOM	343	CB	VAL	46	10.076	13.715	21.179
	1.00	8.74						
45	ATOM	344	CG1	VAL	46	8.860	12.823	20.921
	1.00	9.06						
	ATOM	345	CG2	VAL	46	10.226	13.721	22.656
	1.00	8.48						
	ATOM	346	C	VAL	46	11.179	13.174	19.034
50	1.00	9.06						
	ATOM	347	O	VAL	46	11.069	14.250	18.422
	1.00	7.02						
	ATOM	348	N	ALA	47	11.148	11.984	18.423
	1.00	10.19						
55	ATOM	349	CA	ALA	47	11.088	11.923	16.970
	1.00	11.40						

	ATOM	350	CB	ALA	47	12.487	11.628	16.548
	1.00	14.35						
	ATOM	351	C	ALA	47	10.115	10.894	16.379
	1.00	11.87						
5	ATOM	352	O	ALA	47	10.126	9.770	16.905
	1.00	11.08						
	ATOM	353	N	GLY	48	9.315	11.134	15.349
	1.00	9.25						
	ATOM	354	CA	GLY	48	8.396	10.089	14.949
10	1.00	11.87						
	ATOM	355	C	GLY	48	7.493	10.425	13.794
	1.00	11.00						
	ATOM	356	O	GLY	48	7.513	11.559	13.316
	1.00	11.18						
15	ATOM	357	N	LYS	49	6.712	9.448	13.324
	1.00	9.47						
	ATOM	358	CA	LYS	49	5.783	9.700	12.233
	1.00	8.49						
	ATOM	359	CB	LYS	49	6.156	8.995	10.959
20	1.00	7.23						
	ATOM	360	CG	LYS	49	7.203	9.663	10.124
	1.00	7.71						
	ATOM	361	CD	LYS	49	7.411	8.921	8.809
	1.00	8.83						
25	ATOM	362	CE	LYS	49	8.141	9.814	7.800
	1.00	9.61						
	ATOM	363	NZ	LYS	49	8.376	9.080	6.554
	1.00	11.96						
	ATOM	364	C	LYS	49	4.398	9.237	12.597
30	1.00	8.57						
	ATOM	365	O	LYS	49	4.248	8.384	13.486
	1.00	9.28						
	ATOM	366	N	GLY	50	3.361	9.766	11.960
	1.00	8.33						
35	ATOM	367	CA	GLY	50	2.000	9.425	12.301
	1.00	8.35						
	ATOM	368	C	GLY	50	0.963	10.342	11.663
	1.00	10.55						
	ATOM	369	O	GLY	50	0.966	10.545	10.442
40	1.00	10.22						
	ATOM	370	N	TRP	51	0.070	10.906	12.511
	1.00	11.01						
	ATOM	371	CA	TRP	51	-1.118	11.652	12.085
	1.00	12.06						
45	ATOM	372	CB	TRP	51	-2.423	10.864	12.333
	1.00	11.79						
	ATOM	373	CG	TRP	51	-2.333	9.504	11.635
	1.00	13.30						
	ATOM	374	CD2	TRP	51	-1.674	8.392	12.124
50	1.00	13.13						
	ATOM	375	CE2	TRP	51	-1.810	7.489	11.080
	1.00	14.19						
	ATOM	376	CE3	TRP	51	-0.996	8.040	13.282
	1.00	12.35						
55	ATOM	377	CD1	TRP	51	-2.848	9.301	10.393
	1.00	13.99						

	ATOM	378	NE1	TRP	51	-2.494	8.051	10.078
	1.00	14.34						
	ATOM	379	CZ2	TRP	51	-1.271	6.217	11.162
	1.00	15.05						
5	ATOM	380	CZ3	TRP	51	-0.457	6.769	13.365
	1.00	14.41						
	ATOM	381	CH2	TPP	51	-0.595	5.873	12.316
	1.00	14.24						
10	ATOM	382	C	TRP	51	-1.291	12.983	12.788
	1.00	11.13						
	ATOM	383	O	TRP	51	-0.968	13.135	13.964
	1.00	9.97						
	ATOM	384	N	GLN	52	-1.795	13.962	12.028
	1.00	13.14						
15	ATOM	385	CA	GLN	52	-2.174	15.267	12.560
	1.00	14.01						
	ATOM	386	CB	GLN	52	-1.088	16.284	12.168
	1.00	13.62						
20	ATOM	387	CG	GLN	52	-1.328	17.699	12.606
	1.00	15.07						
	ATOM	388	CD	GLN	52	-1.494	17.915	14.104
	1.00	14.27						
	ATOM	389	OE1	GLN	52	-0.629	18.407	14.830
	1.00	16.02						
25	ATOM	390	NE2	GLN	52	-2.657	17.626	14.635
	1.00	13.08						
	ATOM	391	C	GLN	52	-3.559	15.701	12.054
	1.00	13.05						
	ATOM	392	O	GLN	52	-3.704	16.030	10.868
30	1.00	14.72						
	ATOM	393	N	PRO	53	-4.628	15.721	12.866
	1.00	13.11						
	ATOM	394	CD	PRO	53	-5.967	16.150	12.469
	1.00	13.04						
35	ATOM	395	CA	PRO	53	-4.680	15.205	14.223
	1.00	12.06						
	ATOM	396	CB	PRO	53	-5.876	15.851	14.828
	1.00	12.56						
40	ATOM	397	CG	PRO	53	-6.846	15.722	13.670
	1.00	12.67						
	ATOM	398	C	PRO	53	-4.799	13.691	14.254
	1.00	12.14						
	ATOM	399	O	PRO	53	-5.135	13.011	13.248
	1.00	10.91						
45	ATOM	400	N	GLY	54	-4.607	13.246	15.484
	1.00	12.13						
	ATOM	401	CA	GLY	54	-4.869	11.866	15.739
	1.00	13.75						
	ATOM	402	C	GLY	54	-6.346	11.663	16.041
50	1.00	15.01						
	ATOM	403	O	GLY	54	-7.172	12.582	16.005
	1.00	15.77						
	ATOM	404	N	THR	55	-6.740	10.453	16.400
	1.00	15.56						
55	ATOM	405	CA	THR	55	-8.135	10.178	16.694
	1.00	16.04						

	ATOM	406	CB	THR	55	-8.827	9.410	15.572
	1.00	15.48						
	ATOM	407	OG1	THR	55	-8.200	8.132	15.474
	1.00	15.49						
5	ATOM	408	CG2	THR	55	-8.800	10.183	14.265
	1.00	15.96						
	ATOM	409	C	THR	55	-8.258	9.350	17.937
	1.00	16.77						
10	ATOM	410	O	THR	55	-7.322	8.644	18.310
	1.00	16.68						
	ATOM	411	N	LYS	56	-9.438	9.279	18.531
	1.00	19.29						
	ATOM	412	CA	LYS	56	-9.564	8.452	19.725
	1.00	21.92						
15	ATOM	413	CB	LYS	56	-10.675	9.096	20.595
	1.00	23.92						
	ATOM	414	CG	LYS	56	-10.234	10.565	20.893
	1.00	26.95						
20	ATOM	415	CD	LYS	56	-10.828	11.213	22.151
	1.00	29.47						
	ATOM	416	CE	LYS	56	-10.528	12.739	22.187
	1.00	31.18						
	ATOM	417	NZ	LYS	56	-10.775	13.356	23.492
	1.00	32.24						
25	ATOM	418	C	LYS	56	-9.831	6.988	19.365
	1.00	22.96						
	ATOM	419	O	LYS	56	-10.122	6.137	20.230
	1.00	24.28						
30	ATOM	420	N	ASN	57	-9.656	6.581	18.102
	1.00	22.55						
	ATOM	421	CA	ASN	57	-10.009	5.214	17.735
	1.00	22.75						
	ATOM	422	CB	ASN	57	-11.479	5.164	17.184
	1.00	24.35						
35	ATOM	423	CG	ASN	57	-11.671	5.923	15.848
	1.00	27.06						
	ATOM	424	OD1	ASN	57	-11.050	6.960	15.544
	1.00	27.62						
40	ATOM	425	ND2	ASN	57	-12.539	5.461	14.955
	1.00	27.78						
	ATOM	426	C	ASN	57	-9.048	4.680	16.679
	1.00	21.44						
	ATOM	427	O	ASN	57	-9.397	3.777	15.896
	1.00	22.71						
45	ATOM	428	N	LYS	58	-7.821	5.193	16.624
	1.00	18.17						
	ATOM	429	CA	LYS	58	-6.950	4.785	15.552
	1.00	15.67						
50	ATOM	430	CB	LYS	58	-5.911	5.860	15.363
	1.00	16.07						
	ATOM	431	CG	LYS	58	-5.278	5.787	13.998
	1.00	17.83						
	ATOM	432	CD	LYS	58	-4.526	7.069	13.607
	1.00	18.91						
55	ATOM	433	CE	LYS	58	-5.410	8.299	13.205
	1.00	18.54						

	ATOM	434	NZ	LYS	58	-6.249	8.140	11.995
	1.00	19.60						
	ATOM	435	C	LYS	58	-6.334	3.476	15.978
	1.00	13.93						
5	ATOM	436	O	LYS	58	-6.086	3.300	17.171
	1.00	15.02						
	ATOM	437	N	VAL	59	-6.174	2.474	15.131
	1.00	13.40						
10	ATOM	438	CA	VAL	59	-5.364	1.313	15.506
	1.00	12.92						
	ATOM	439	CB	VAL	59	-6.203	-0.053	15.388
	1.00	14.48						
	ATOM	440	CG1	VAL	59	-7.120	-0.117	14.200
	1.00	16.35						
15	ATOM	441	CG2	VAL	59	-5.192	-1.198	15.311
	1.00	13.23						
	ATOM	442	C	VAL	59	-4.138	1.408	14.583
	1.00	11.86						
20	ATOM	443	O	VAL	59	-4.167	1.542	13.343
	1.00	12.38						
	ATOM	444	N	ILE	60	-3.061	1.577	15.346
	1.00	10.27						
	ATOM	445	CA	ILE	60	-1.749	1.915	14.826
	1.00	9.01						
25	ATOM	446	CB	ILE	60	-1.119	3.011	15.700
	1.00	8.58						
	ATOM	447	CG2	ILE	60	0.280	3.326	15.213
	1.00	8.04						
30	ATOM	448	CG1	ILE	60	-2.000	4.252	15.663
	1.00	7.60						
	ATOM	449	CD1	ILE	60	-1.611	5.192	16.759
	1.00	9.90						
	ATOM	450	C	ILE	60	-0.851	0.725	14.800
	1.00	9.88						
35	ATOM	451	O	ILE	60	-0.680	0.059	15.822
	1.00	9.11						
	ATOM	452	N	ASN	61	-0.270	0.546	13.616
	1.00	11.11						
40	ATOM	453	CA	ASN	61	0.671	-0.545	13.341
	1.00	10.36						
	ATOM	454	CB	ASN	61	0.366	-1.204	12.006
	1.00	12.63						
	ATOM	455	CG	ASN	61	-1.072	-1.619	11.996
	1.00	14.76						
45	ATOM	456	OD1	ASN	61	-1.478	-2.378	12.874
	1.00	16.78						
	ATOM	457	ND2	ASN	61	-1.921	-1.111	11.095
	1.00	15.45						
50	ATOM	458	C	ASN	61	2.088	-0.032	13.291
	1.00	9.66						
	ATOM	459	O	ASN	61	2.338	1.095	12.867
	1.00	9.13						
	ATOM	460	N	PHE	62	3.042	-0.806	13.765
	1.00	9.56						
55	ATOM	461	CA	PHE	62	4.422	-0.405	13.688
	1.00	10.44						

	ATOM	462	CB	PHE	62	4.865	0.454	14.933
	1.00	9.48						
	ATOM	463	CG	PHE	62	4.657	-0.145	16.314
	1.00	9.74						
5	ATOM	464	CD1	PHE	62	5.751	-0.618	17.021
	1.00	10.19						
	ATOM	465	CD2	PHE	62	3.371	-0.259	16.828
	1.00	10.24						
10	ATOM	466	CE1	PHE	62	5.546	-1.224	18.250
	1.00	9.20						
	ATOM	467	CE2	PHE	62	3.176	-0.867	18.054
	1.00	9.66						
	ATOM	468	CZ	PHE	62	4.274	-1.347	18.757
	1.00	9.91						
15	ATOM	469	C	PHE	62	5.348	-1.590	13.570
	1.00	9.69						
	ATOM	470	O	PHE	62	5.066	-2.608	14.200
	1.00	11.84						
20	ATOM	471	N	SER	63	6.404	-1.538	12.767
	1.00	11.03						
	ATOM	472	CA	SER	63	7.449	-2.547	12.847
	1.00	11.59						
	ATOM	473	CB	SER	63	7.328	-3.650	11.765
	1.00	12.00						
25	ATOM	474	OG	SER	63	7.114	-3.195	10.463
	1.00	12.51						
	ATOM	475	C	SER	63	8.819	-1.923	12.715
	1.00	11.22						
	ATOM	476	O	SER	63	8.928	-0.727	12.379
30	1.00	12.00						
	ATOM	477	N	GLY	64	9.823	-2.781	12.942
	1.00	10.23						
	ATOM	478	CA	GLY	64	11.193	-2.372	12.823
	1.00	8.33						
35	ATOM	479	C	GLY	64	11.988	-2.761	14.029
	1.00	7.41						
	ATOM	480	O	GLY	64	11.615	-3.676	14.751
	1.00	8.00						
40	ATOM	481	N	SER	65	13.077	-2.058	14.222
	1.00	7.92						
	ATOM	482	CA	SER	65	13.961	-2.346	15.314
	1.00	10.77						
	ATOM	483	CB	SER	65	15.240	-2.865	14.680
	1.00	12.34						
45	ATOM	484	OG	SER	65	15.702	-2.010	13.636
	1.00	12.01						
	ATOM	485	C	SER	65	14.215	-1.151	16.250
	1.00	10.66						
	ATOM	486	O	SER	65	14.393	-0.010	15.791
50	1.00	11.27						
	ATOM	487	N	TYR	66	14.338	-1.407	17.535
	1.00	8.76						
	ATOM	488	CA	TYR	66	14.573	-0.359	18.514
	1.00	8.36						
55	ATOM	489	CB	TYR	66	13.258	-0.091	19.279
	1.00	6.60						

	ATOM	490	CG	TYR	66	13.429	0.738	20.539
	1.00	5.88						
	ATOM	491	CD1	TYR	66	13.005	0.198	21.732
	1.00	3.88						
5	ATOM	492	CE1	TYR	66	13.053	0.928	22.894
	1.00	3.78						
	ATOM	493	CD2	TYR	66	13.932	2.032	20.506
	1.00	5.67						
10	ATOM	494	CE2	TYR	66	13.982	2.780	21.677
	1.00	3.65						
	ATOM	495	CZ	TYR	66	13.533	2.217	22.851
	1.00	4.38						
	ATOM	496	OH	TYR	66	13.501	2.961	24.006
	1.00	5.96						
15	ATOM	497	C	TYR	66	15.667	-0.905	19.416
	1.00	8.49						
	ATOM	498	O	TYR	66	15.539	-1.954	20.045
	1.00	8.59						
20	ATOM	499	N	ASN	67	16.768	-0.197	19.470
	1.00	10.09						
	ATOM	500	CA	ASN	67	17.951	-0.686	20.156
	1.00	11.81						
	ATOM	501	CB	ASN	67	18.968	-1.158	19.130
	1.00	15.94						
25	ATOM	502	CG	ASN	67	18.427	-2.110	18.028
	1.00	20.43						
	ATOM	503	OD1	ASN	67	18.079	-3.269	18.260
	1.00	21.28						
30	ATOM	504	ND2	ASN	67	18.287	-1.681	16.767
	1.00	22.48						
	ATOM	505	C	ASN	67	18.556	0.438	21.016
	1.00	11.16						
	ATOM	506	O	ASN	67	19.512	1.103	20.618
	1.00	8.26						
35	ATOM	507	N	PRO	68	17.937	0.733	22.173
	1.00	10.94						
	ATOM	508	CD	PRO	68	16.694	0.131	22.659
	1.00	10.82						
40	ATOM	509	CA	PRO	68	18.378	1.755	23.099
	1.00	11.97						
	ATOM	510	CB	PRO	68	17.103	2.066	23.890
	1.00	11.53						
	ATOM	511	CG	PRO	68	16.437	0.732	24.019
	1.00	10.89						
45	ATOM	512	C	PRO	68	19.561	1.340	23.957
	1.00	11.57						
	ATOM	513	O	PRO	68	19.689	0.209	24.442
	1.00	10.78						
50	ATOM	514	N	ASN	69	20.429	2.277	24.207
	1.00	9.77						
	ATOM	515	CA	ASN	69	21.523	2.025	25.094
	1.00	11.79						
	ATOM	516	CB	ASN	69	22.744	2.036	24.242
	1.00	13.60						
55	ATOM	517	CG	ASN	69	23.967	1.656	25.041
	1.00	17.40						

	ATOM	518	OD1	ASN	69	25.063	1.812	24.504
	1.00	21.47						
	ATOM	519	ND2	ASN	69	24.006	1.089	26.244
	1.00	17.05						
5	ATOM	520	C	ASN	69	21.484	3.117	26.179
	1.00	12.60						
	ATOM	521	O	ASN	69	22.208	4.144	26.160
	1.00	13.38						
10	ATOM	522	N	GLY	70	20.491	2.932	27.046
	1.00	8.91						
	ATOM	523	CA	GLY	70	20.226	3.850	28.114
	1.00	8.37						
	ATOM	524	C	GLY	70	18.795	4.357	28.073
	1.00	8.21						
15	ATOM	525	O	GLY	70	17.842	3.663	27.670
	1.00	9.06						
	ATOM	526	N	ASN	71	18.656	5.595	28.502
	1.00	7.03						
20	ATOM	527	CA	ASN	71	17.347	6.161	28.701
	1.00	7.69						
	ATOM	528	CB	ASN	71	17.448	7.409	29.589
	1.00	7.29						
	ATOM	529	CG	ASN	71	16.104	7.886	30.142
	1.00	8.85						
25	ATOM	530	OD1	ASN	71	15.032	7.684	29.577
	1.00	9.56						
	ATOM	531	ND2	ASN	71	16.047	8.491	31.329
	1.00	7.50						
30	ATOM	532	C	ASN	71	16.668	6.525	27.391
	1.00	8.37						
	ATOM	533	O	ASN	71	17.072	7.537	26.762
	1.00	9.29						
	ATOM	534	N	SER	72	15.643	5.733	27.043
	1.00	6.66						
35	ATOM	535	CA	SER	72	14.864	5.953	25.837
	1.00	7.05						
	ATOM	536	CB	SER	72	15.699	5.398	24.662
	1.00	7.68						
40	ATOM	537	OG	SER	72	15.191	5.543	23.349
	1.00	8.77						
	ATOM	538	C	SER	72	13.483	5.286	25.932
	1.00	8.50						
	ATOM	539	O	SER	72	13.292	4.335	26.722
	1.00	8.19						
45	ATOM	540	N	TYR	73	12.520	5.701	25.110
	1.00	7.79						
	ATOM	541	CA	TYR	73	11.190	5.154	25.058
	1.00	7.74						
50	ATOM	542	CB	TYR	73	10.094	6.073	25.659
	1.00	7.66						
	ATOM	543	CG	TYR	73	10.319	6.583	27.099
	1.00	10.11						
	ATOM	544	CD1	TYR	73	10.919	5.817	28.103
	1.00	9.07						
55	ATOM	545	CE1	TYR	73	11.121	6.358	29.366
	1.00	9.86						



	ATOM	546	CD2	TYR	73	9.920	7.881	27.376
	1.00	10.46						
	ATOM	547	CE2	TYR	73	10.116	8.418	28.625
	1.00	9.86						
5	ATOM	548	CZ	TYR	73	10.709	7.668	29.607
	1.00	10.88						
	ATOM	549	OH	TYR	73	10.868	8.246	30.846
	1.00	10.66						
10	ATOM	550	C	TYR	73	10.796	4.932	23.600
	1.00	8.12						
	ATOM	551	O	TYR	73	11.244	5.627	22.676
	1.00	8.31						
	ATOM	552	N	LEU	74	9.946	3.942	23.394
	1.00	6.70						
15	ATOM	553	CA	LEU	74	9.292	3.736	22.104
	1.00	7.34						
	ATOM	554	CB	LEU	74	9.677	2.388	21.485
	1.00	7.37						
20	ATOM	555	CG	LEU	74	8.939	1.937	20.190
	1.00	8.67						
	ATOM	556	CD1	LEU	74	9.182	2.886	19.023
	1.00	8.01						
	ATOM	557	CD2	LEU	74	9.430	0.523	19.850
	1.00	8.15						
25	ATOM	558	C	LEU	74	7.805	3.752	22.500
	1.00	6.80						
	ATOM	559	O	LEU	74	7.359	2.918	23.297
	1.00	6.53						
30	ATOM	560	N	SER	75	7.030	4.688	21.973
	1.00	5.87						
	ATOM	561	CA	SER	75	5.669	4.839	22.425
	1.00	5.53						
	ATOM	562	CB	SER	75	5.555	5.907	23.516
	1.00	6.86						
35	ATOM	563	OG	SER	75	6.582	5.955	24.476
	1.00	11.37						
	ATOM	564	C	SER	75	4.770	5.295	21.297
	1.00	4.71						
40	ATOM	565	O	SER	75	5.235	5.772	20.263
	1.00	4.19						
	ATOM	566	N	ILE	76	3.485	5.121	21.489
	1.00	3.93						
	ATOM	567	CA	ILE	76	2.508	5.857	20.711
	1.00	5.49						
45	ATOM	568	CB	ILE	76	1.190	5.090	20.679
	1.00	7.40						
	ATOM	569	CG2	ILE	76	0.068	6.005	20.340
	1.00	8.03						
50	ATOM	570	CG1	ILE	76	1.184	4.029	19.557
	1.00	8.58						
	ATOM	571	CD1	ILE	76	2.241	2.921	19.633
	1.00	9.45						
	ATOM	572	C	ILE	76	2.465	7.108	21.600
	1.00	6.93						
55	ATOM	573	O	ILE	76	2.370	6.973	22.829
	1.00	7.49						

	ATOM	574	N	TYR	77	2.627	8.295	21.020
	1.00	6.57						
	ATOM	575	CA	TYR	77	2.811	9.555	21.724
	1.00	5.67						
5	ATOM	576	CB	TYR	77	4.299	9.948	21.647
	1.00	4.54						
	ATOM	577	CG	TYR	77	4.686	11.364	22.139
	1.00	4.19						
	ATOM	578	CD1	TYR	77	4.668	11.654	23.497
10	1.00	4.75						
	ATOM	579	CE1	TYR	77	4.991	12.901	23.966
	1.00	4.71						
	ATOM	580	CD2	TYR	77	5.044	12.363	21.240
	1.00	4.76						
15	ATOM	581	CE2	TYR	77	5.373	13.638	21.694
	1.00	3.95						
	ATOM	582	CZ	TYR	77	5.341	13.894	23.060
	1.00	5.09						
	ATOM	583	OH	TYR	77	5.641	15.159	23.541
20	1.00	6.11						
	ATOM	584	C	TYR	77	1.961	10.639	21.098
	1.00	5.81						
	ATOM	585	O	TYR	77	1.888	10.741	19.856
	1.00	6.39						
25	ATOM	586	N	GLY	78	1.359	11.509	21.898
	1.00	5.96						
	ATOM	587	CA	GLY	78	0.615	12.588	21.278
	1.00	6.69						
	ATOM	588	C	GLY	78	0.156	13.586	22.288
30	1.00	7.28						
	ATOM	589	O	GLY	78	0.537	13.494	23.466
	1.00	7.84						
	ATOM	590	N	TRP	79	-0.672	14.528	21.822
	1.00	7.76						
35	ATOM	591	CA	TRP	79	-1.234	15.560	22.707
	1.00	7.51						
	ATOM	592	CB	TRP	79	-0.598	16.949	22.555
	1.00	6.56						
	ATOM	593	CG	TRP	79	0.876	17.041	22.832
40	1.00	5.50						
	ATOM	594	CD2	TRP	79	1.419	17.620	23.935
	1.00	5.87						
	ATOM	595	CE2	TRP	79	2.774	17.469	23.695
	1.00	5.84						
45	ATOM	596	CE3	TRP	79	0.951	18.249	25.072
	1.00	5.83						
	ATOM	597	CD1	TRP	79	1.819	16.560	21.962
	1.00	6.72						
	ATOM	598	NE1	TRP	79	2.963	16.842	22.524
50	1.00	5.73						
	ATOM	599	CZ2	TRP	79	3.695	17.950	24.600
	1.00	5.70						
	ATOM	600	CZ3	TRP	79	1.867	18.733	25.972
	1.00	5.50						
55	ATOM	601	CH2	TRP	79	3.226	18.581	25.742
	1.00	5.81						

	ATOM	602	C	TRP	79	-2.702	15.796	22.434
	1.00	7.13						
	ATOM	603	O	TRP	79	-3.219	15.434	21.365
	1.00	6.19						
5	ATOM	604	N	SER	80	-3.360	16.381	23.440
	1.00	8.56						
	ATOM	605	CA	SER	80	-4.683	16.933	23.242
	1.00	11.11						
10	ATOM	606	CB	SER	80	-5.761	16.138	23.974
	1.00	10.43						
	ATOM	607	OG	SER	80	-5.890	16.355	25.385
	1.00	16.05						
	ATOM	608	C	SER	80	-4.643	18.381	23.781
	1.00	10.31						
15	ATOM	609	O	SER	80	-3.732	18.753	24.528
	1.00	9.07						
	ATOM	610	N	ARG	81	-5.593	19.225	23.392
	1.00	12.84						
20	ATOM	611	CA	ARG	81	-5.732	20.562	23.953
	1.00	15.11						
	ATOM	612	CB	ARG	81	-5.614	21.564	22.851
	1.00	18.41						
	ATOM	613	CG	ARG	81	-4.205	21.639	22.307
	1.00	22.70						
25	ATOM	614	CD	ARG	81	-4.381	22.114	20.897
	1.00	25.52						
	ATOM	615	NE	ARG	81	-3.063	22.554	20.439
	1.00	29.78						
30	ATOM	616	CZ	ARG	81	-2.811	22.897	19.179
	1.00	30.17						
	ATOM	617	NH1	ARG	81	-3.810	22.847	18.270
	1.00	32.23						
	ATOM	618	NH2	ARG	81	-1.547	23.168	18.822
	1.00	30.78						
35	ATOM	619	C	ARG	81	-7.071	20.736	24.659
	1.00	13.57						
	ATOM	620	O	ARG	81	-8.067	20.129	24.261
	1.00	12.68						
40	ATOM	621	N	ASN	82	-7.100	21.628	25.667
	1.00	13.97						
	ATOM	622	CA	ASN	82	-8.284	21.968	26.448
	1.00	13.79						
	ATOM	623	CB	ASN	82	-9.250	22.793	25.588
	1.00	14.31						
45	ATOM	624	CG	ASN	82	-8.645	24.103	25.115
	1.00	15.90						
	ATOM	625	OD1	ASN	82	-8.695	24.391	23.929
	1.00	18.55						
	ATOM	626	ND2	ASN	82	-7.998	24.954	25.904
50	1.00	16.49						
	ATOM	627	C	ASN	82	-9.012	20.744	27.004
	1.00	13.02						
	ATOM	628	O	ASN	82	-10.109	20.409	26.570
	1.00	13.95						
55	ATOM	629	N	PRO	83	-8.490	19.988	27.956
	1.00	11.90						

	ATOM	630	CD	PRO	83	-9.129	18.759	28.468
	1.00	12.28						
	ATOM	631	CA	PRO	83	-7.228	20.233	28.616
	1.00	10.88						
5	ATOM	632	CB	PRO	83	-7.374	19.477	29.921
	1.00	11.28						
	ATOM	633	CG	PRO	83	-8.168	18.254	29.514
	1.00	12.43						
10	ATOM	634	C	PRO	83	-6.020	19.812	27.806
	1.00	9.55						
	ATOM	635	O	PRO	83	-6.065	18.925	26.941
	1.00	10.93						
	ATOM	636	N	LEU	84	-4.949	20.487	28.139
	1.00	9.55						
15	ATOM	637	CA	LEU	84	-3.650	20.212	27.575
	1.00	10.04						
	ATOM	638	CB	LEU	84	-2.725	21.373	27.908
	1.00	9.09						
20	ATOM	639	CG	LEU	84	-1.343	21.354	27.288
	1.00	9.70						
	ATOM	640	CD1	LEU	84	-1.402	21.496	25.777
	1.00	8.76						
	ATOM	641	CD2	LEU	84	-0.580	22.526	27.836
	1.00	10.04						
25	ATOM	642	C	LEU	84	-3.170	18.903	28.205
	1.00	9.91						
	ATOM	643	O	LEU	84	-3.002	18.839	29.428
	1.00	10.98						
30	ATOM	644	N	ILE	85	-2.966	17.863	27.375
	1.00	10.87						
	ATOM	645	CA	ILE	85	-2.538	16.538	27.873
	1.00	11.93						
	ATOM	646	CB	ILE	85	-3.711	15.489	27.812
	1.00	11.72						
35	ATOM	647	CG2	ILE	85	-3.226	14.128	28.360
	1.00	12.89						
	ATOM	648	CG1	ILE	85	-4.909	15.932	28.663
	1.00	11.57						
40	ATOM	649	CD1	ILE	85	-4.578	16.047	30.178
	1.00	11.61						
	ATOM	650	C	ILE	85	-1.393	16.023	27.028
	1.00	10.50						
	ATOM	651	O	ILE	85	-1.481	16.104	25.799
	1.00	12.37						
45	ATOM	652	N	GLU	86	-0.310	15.580	27.654
	1.00	10.70						
	ATOM	653	CA	GLU	86	0.725	14.868	26.909
	1.00	10.27						
50	ATOM	654	CB	GLU	86	2.072	15.269	27.364
	1.00	8.12						
	ATOM	655	CG	GLU	86	3.207	14.580	26.675
	1.00	6.80						
	ATOM	656	CD	GLU	86	4.537	15.107	27.134
	1.00	8.51						
55	ATOM	657	OE1	GLU	86	5.414	15.338	26.303
	1.00	9.55						

	ATOM	658	OE2	GLU	86	4.717	15.329	28.333
	1.00	11.97						
	ATOM	659	C	GLU	86	0.491	13.405	27.268
	1.00	9.41						
5	ATOM	660	O	GLU	86	0.386	13.100	28.464
	1.00	10.26						
	ATOM	661	N	TYR	87	0.324	12.484	26.315
	1.00	7.81						
10	ATOM	662	CA	TYR	87	0.083	11.088	26.705
	1.00	7.22						
	ATOM	663	CB	TYR	87	-1.380	10.679	26.368
	1.00	5.93						
	ATOM	664	CG	TYR	87	-1.738	10.658	24.884
	1.00	7.18						
15	ATOM	665	CD1	TYR	87	-1.474	9.535	24.099
	1.00	8.82						
	ATOM	666	CE1	TYR	87	-1.766	9.541	22.758
	1.00	7.19						
20	ATOM	667	CD2	TYR	87	-2.307	11.750	24.278
	1.00	6.85						
	ATOM	668	CE2	TYR	87	-2.612	11.756	22.941
	1.00	5.57						
	ATOM	669	CZ	TYR	87	-2.335	10.650	22.181
	1.00	7.53						
25	ATOM	670	OH	TYR	87	-2.601	10.636	20.820
	1.00	7.92						
	ATOM	671	C	TYR	87	1.089	10.145	26.007
	1.00	7.60						
30	ATOM	672	O	TYR	87	1.593	10.460	24.914
	1.00	6.22						
	ATOM	673	N	TYR	88	1.277	8.961	26.612
	1.00	7.31						
	ATOM	674	CA	TYR	88	2.217	7.936	26.154
	1.00	7.56						
35	ATOM	675	CB	TYR	88	3.528	7.871	26.929
	1.00	7.13						
	ATOM	676	CG	TYR	88	4.468	9.042	27.007
	1.00	8.10						
40	ATOM	677	CD1	TYR	88	4.116	10.234	27.638
	1.00	7.71						
	ATOM	678	CE1	TYR	88	5.051	11.255	27.679
	1.00	9.49						
	ATOM	679	CD2	TYR	88	5.718	8.892	26.443
	1.00	9.02						
45	ATOM	680	CE2	TYR	88	6.648	9.911	26.481
	1.00	9.73						
	ATOM	681	CZ	TYR	88	6.293	11.080	27.099
	1.00	8.95						
50	ATOM	682	OH	TYR	88	7.201	12.087	27.106
	1.00	10.51						
	ATOM	683	C	TYR	88	1.650	6.523	26.351
	1.00	8.02						
	ATOM	684	O	TYR	88	1.044	6.170	27.392
	1.00	9.02						
55	ATOM	685	N	ILE	89	1.732	5.702	25.323
	1.00	8.56						

	ATOM	686	CA	ILE	89	1.416	4.327	25.590
	1.00	8.75						
	ATOM	687	CB	ILE	89	0.027	3.839	24.820
	1.00	11.11						
5	ATOM	688	CG2	ILE	89	-1.015	4.940	24.514
	1.00	11.61						
	ATOM	689	CG1	ILE	89	0.325	3.284	23.516
	1.00	14.51						
10	ATOM	690	CD1	ILE	89	0.188	1.799	23.814
	1.00	14.55						
	ATOM	691	C	ILE	89	2.753	3.699	25.133
	1.00	7.56						
	ATOM	692	O	ILE	89	3.184	3.694	23.968
	1.00	7.22						
15	ATOM	693	N	VAL	90	3.532	3.345	26.134
	1.00	5.27						
	ATOM	694	CA	VAL	90	4.871	2.849	25.887
	1.00	7.56						
20	ATOM	695	CB	VAL	90	5.825	3.471	27.042
	1.00	8.16						
	ATOM	696	CG1	VAL	90	5.051	3.700	28.284
	1.00	11.52						
	ATOM	697	CG2	VAL	90	7.017	2.585	27.388
	1.00	9.08						
25	ATOM	698	C	VAL	90	4.978	1.309	25.703
	1.00	7.15						
	ATOM	699	O	VAL	90	4.665	0.486	26.563
	1.00	5.67						
30	ATOM	700	N	GLU	91	5.408	0.986	24.489
	1.00	7.73						
	ATOM	701	CA	GLU	91	5.615	-0.376	24.005
	1.00	6.96						
	ATOM	702	CB	GLU	91	5.524	-0.319	22.468
	1.00	6.72						
35	ATOM	703	CG	GLU	91	4.117	0.109	21.997
	1.00	6.68						
	ATOM	704	CD	GLU	91	2.997	-0.826	22.456
	1.00	7.56						
40	ATOM	705	OE1	GLU	91	2.351	-0.578	23.452
	1.00	6.34						
	ATOM	706	OE2	GLU	91	2.725	-1.823	21.810
	1.00	7.24						
	ATOM	707	C	GLU	91	6.930	-1.017	24.472
	1.00	8.03						
45	ATOM	708	O	GLU	91	7.030	-2.224	24.753
	1.00	8.58						
	ATOM	709	N	ASN	92	7.982	-0.202	24.624
	1.00	6.40						
50	ATOM	710	CA	ASN	92	9.301	-0.640	24.993
	1.00	5.56						
	ATOM	711	CB	ASN	92	9.971	-1.242	23.777
	1.00	7.20						
	ATOM	712	CG	ASN	92	11.086	-2.249	24.078
	1.00	4.55						
55	ATOM	713	OD1	ASN	92	11.508	-2.921	23.158
	1.00	8.31						

	ATOM	714	ND2	ASN	92	11.658	-2.485	25.235
	1.00	4.54						
	ATOM	715	C	ASN	92	10.101	0.567	25.492
	1.00	6.87						
5	ATOM	716	O	ASN	92	9.730	1.715	25.226
	1.00	6.30						
	ATOM	717	N	PHE	93	11.178	0.358	26.247
	1.00	6.43						
10	ATOM	718	CA	PHE	93	12.014	1.435	26.793
	1.00	7.21						
	ATOM	719	CB	PHE	93	11.316	2.114	27.994
	1.00	5.14						
	ATOM	720	CG	PHE	93	10.879	1.272	29.174
	1.00	5.75						
15	ATOM	721	CD1	PHE	93	11.782	0.935	30.168
	1.00	5.51						
	ATOM	722	CD2	PHE	93	9.551	0.889	29.272
	1.00	5.97						
20	ATOM	723	CE1	PHE	93	11.341	0.209	31.274
	1.00	6.76						
	ATOM	724	CE2	PHE	93	9.115	0.163	30.383
	1.00	6.85						
	ATOM	725	CZ	PHE	93	10.013	-0.176	31.378
	1.00	6.45						
25	ATOM	726	C	PHE	93	13.343	0.843	27.218
	1.00	7.46						
	ATOM	727	O	PHE	93	13.439	-0.393	27.217
	1.00	8.45						
30	ATOM	728	N	GLY	94	14.326	1.659	27.611
	1.00	9.27						
	ATOM	729	CA	GLY	94	15.674	1.230	27.935
	1.00	9.67						
	ATOM	730	C	GLY	94	15.826	1.048	29.440
	1.00	10.54						
35	ATOM	731	O	GLY	94	14.938	0.537	30.111
	1.00	11.63						
	ATOM	732	N	THR	95	16.920	1.556	29.966
	1.00	8.02						
40	ATOM	733	CA	THR	95	17.305	1.389	31.345
	1.00	9.56						
	ATOM	734	CB	THR	95	18.812	1.747	31.485
	1.00	10.30						
	ATOM	735	OG1	THR	95	18.950	3.144	31.160
	1.00	12.79						
45	ATOM	736	CG2	THR	95	19.687	0.913	30.581
	1.00	11.07						
	ATOM	737	C	THR	95	16.493	2.215	32.339
	1.00	9.93						
50	ATOM	738	O	THR	95	16.646	2.037	33.545
	1.00	7.89						
	ATOM	739	N	TYR	96	15.683	3.177	31.892
	1.00	9.40						
	ATOM	740	CA	TYR	96	15.008	4.021	32.850
	1.00	7.32						
55	ATOM	741	CB	TYR	96	15.273	5.509	32.531
	1.00	8.01						

	ATOM	742	CG	TYR	96	14.506	6.456	33.440
	1.00	8.66						
	ATOM	743	CD1	TYR	96	15.004	6.750	34.690
	1.00	11.35						
5	ATOM	744	CE1	TYR	96	14.312	7.595	35.549
	1.00	12.60						
	ATOM	745	CD2	TYR	96	13.322	7.013	33.043
	1.00	9.65						
	ATOM	746	CE2	TYR	96	12.629	7.862	33.892
10	1.00	12.25						
	ATOM	747	CZ	TYR	96	13.125	8.140	35.144
	1.00	12.02						
	ATOM	748	OH	TYR	96	12.398	8.947	36.037
	1.00	16.30						
15	ATOM	749	C	TYR	96	13.547	3.703	32.772
	1.00	7.36						
	ATOM	750	O	TYR	96	12.891	3.804	31.729
	1.00	7.79						
	ATOM	751	N	ASN	97	13.023	3.350	33.925
20	1.00	6.69						
	ATOM	752	CA	ASN	97	11.637	2.945	33.955
	1.00	8.46						
	ATOM	753	CB	ASN	97	11.378	2.061	35.197
	1.00	6.22						
25	ATOM	754	CG	ASN	97	10.028	1.337	35.187
	1.00	8.71						
	ATOM	755	OD1	ASN	97	9.902	0.092	35.210
	1.00	8.88						
	ATOM	756	ND2	ASN	97	8.950	2.081	35.177
30	1.00	4.75						
	ATOM	757	C	ASN	97	10.775	4.208	33.979
	1.00	9.04						
	ATOM	758	O	ASN	97	10.891	5.009	34.918
	1.00	10.16						
35	ATOM	759	N	PRO	98	9.864	4.383	33.017
	1.00	9.73						
	ATOM	760	CD	PRO	98	9.616	3.413	31.965
	1.00	10.11						
	ATOM	761	CA	PRO	98	8.929	5.503	32.905
40	1.00	11.05						
	ATOM	762	CB	PRO	98	8.134	5.233	31.671
	1.00	10.57						
	ATOM	763	CG	PRO	98	8.894	4.168	30.909
	1.00	11.36						
45	ATOM	764	C	PRO	98	7.999	5.746	34.094
	1.00	12.84						
	ATOM	765	O	PRO	98	7.553	6.881	34.328
	1.00	12.98						
	ATOM	766	N	SER	99	7.635	4.699	34.852
50	1.00	11.41						
	ATOM	767	CA	SER	99	6.808	4.887	36.009
	1.00	12.40						
	ATOM	768	CB	SER	99	6.193	3.565	36.411
	1.00	11.96						
55	ATOM	769	OG	SER	99	7.223	2.731	36.896
	1.00	13.35						

	ATOM	770	C	SER	99	7.561	5.483	37.229
	1.00	13.13						
	ATOM	771	O	SER	99	6.887	5.667	38.238
	1.00	12.90						
5	ATOM	772	N	THR	100	8.872	5.814	37.202
	1.00	12.61						
	ATOM	773	CA	THR	100	9.570	6.319	38.373
	1.00	14.31						
10	ATOM	774	CB	THR	100	11.053	6.616	37.908
	1.00	14.57						
	ATOM	775	OG1	THR	100	11.681	5.381	37.513
	1.00	13.39						
	ATOM	776	CG2	THR	100	11.872	7.330	39.000
	1.00	13.16						
15	ATOM	777	C	THR	100	8.855	7.562	38.979
	1.00	15.95						
	ATOM	778	O	THR	100	8.704	7.778	40.199
	1.00	16.24						
20	ATOM	779	N	GLY	101	8.283	8.459	38.197
	1.00	16.98						
	ATOM	780	CA	GLY	101	7.638	9.603	38.908
	1.00	22.81						
	ATOM	781	C	GLY	101	6.275	9.277	39.557
	1.00	22.53						
25	ATOM	782	O	GLY	101	5.846	9.799	40.603
	1.00	24.30						
	ATOM	783	N	ALA	102	5.687	8.272	38.943
	1.00	21.22						
30	ATOM	784	CA	ALA	102	4.281	8.251	38.892
	1.00	20.59						
	ATOM	785	CB	ALA	102	3.987	7.618	37.568
	1.00	22.27						
	ATOM	786	C	ALA	102	3.361	7.726	39.918
	1.00	20.55						
35	ATOM	787	O	ALA	102	3.672	6.926	40.813
	1.00	21.31						
	ATOM	788	N	THR	103	2.136	8.214	39.718
	1.00	19.36						
40	ATOM	789	CA	THR	103	1.096	7.726	40.572
	1.00	18.69						
	ATOM	790	CB	THR	103	0.225	8.936	40.951
	1.00	19.51						
	ATOM	791	OG1	THR	103	1.084	9.806	41.743
	1.00	20.44						
45	ATOM	792	CG2	THR	103	-1.075	8.498	41.648
	1.00	18.11						
	ATOM	793	C	THR	103	0.371	6.668	39.775
	1.00	16.70						
	ATOM	794	O	THR	103	-0.096	7.016	38.695
50	1.00	15.70						
	ATOM	795	N	LYS	104	0.313	5.418	40.253
	1.00	15.07						
	ATOM	796	CA	LYS	104	-0.377	4.378	39.528
	1.00	14.87						
55	ATOM	797	CB	LYS	104	0.040	2.976	40.009
	1.00	15.19						

	ATOM	798	CG	LYS	104	-0.609	1.894	39.106
	1.00	14.18						
	ATOM	799	CD	LYS	104	-0.270	0.443	39.507
	1.00	13.52						
5	ATOM	800	CE	LYS	104	-1.134	-0.507	38.694
	1.00	13.51						
	ATOM	801	NZ	LYS	104	-0.693	-1.884	38.679
	1.00	14.08						
10	ATOM	802	C	LYS	104	-1.865	4.540	39.739
	1.00	15.06						
	ATOM	803	O	LYS	104	-2.343	4.776	40.852
	1.00	16.27						
	ATOM	804	N	LEU	105	-2.604	4.497	38.663
	1.00	14.64						
15	ATOM	805	CA	LEU	105	-4.012	4.642	38.765
	1.00	16.10						
	ATOM	806	CB	LEU	105	-4.554	5.692	37.835
	1.00	18.74						
20	ATOM	807	CG	LEU	105	-4.239	7.181	38.163
	1.00	21.39						
	ATOM	808	CD1	LEU	105	-2.801	7.479	37.844
	1.00	21.27						
	ATOM	809	CD2	LEU	105	-5.016	8.118	37.214
	1.00	22.30						
25	ATOM	810	C	LEU	105	-4.735	3.403	38.415
	1.00	17.33						
	ATOM	811	O	LEU	105	-5.958	3.403	38.613
	1.00	18.71						
30	ATOM	812	N	GLY	106	-4.142	2.420	37.716
	1.00	16.78						
	ATOM	813	CA	GLY	106	-4.924	1.256	37.323
	1.00	14.69						
	ATOM	814	C	GLY	106	-4.212	0.434	36.268
	1.00	14.81						
35	ATOM	815	O	GLY	106	-2.996	0.602	36.101
	1.00	14.33						
	ATOM	816	N	GLU	107	-4.969	-0.468	35.612
	1.00	14.31						
40	ATOM	817	CA	GLU	107	-4.471	-1.347	34.563
	1.00	14.01						
	ATOM	818	CB	GLU	107	-4.139	-2.724	35.141
	1.00	17.27						
	ATOM	819	CG	GLU	107	-3.101	-2.650	36.288
	1.00	19.43						
45	ATOM	820	CD	GLU	107	-3.045	-3.847	37.242
	1.00	21.27						
	ATOM	821	OE1	GLU	107	-3.493	-4.937	36.863
	1.00	20.90						
	ATOM	822	OE2	GLU	107	-2.507	-3.677	38.362
50	1.00	22.15						
	ATOM	823	C	GLU	107	-5.503	-1.522	33.465
	1.00	12.12						
	ATOM	824	O	GLU	107	-6.703	-1.267	33.664
	1.00	11.04						
55	ATOM	825	N	VAL	108	-5.003	-1.974	32.315
	1.00	11.87						

	ATOM	826	CA	VAL	108	-5.812	-2.265	31.129
	1.00	13.37						
	ATOM	827	CB	VAL	108	-6.069	-0.940	30.283
	1.00	12.75						
5	ATOM	828	CG1	VAL	108	-4.742	-0.406	29.730
	1.00	13.07						
	ATOM	829	CG2	VAL	108	-6.925	-1.184	29.045
	1.00	13.15						
10	ATOM	830	C	VAL	108	-5.034	-3.299	30.306
	1.00	11.86						
	ATOM	831	O	VAL	108	-3.796	-3.269	30.185
	1.00	12.43						
	ATOM	832	N	THR	109	-5.786	-4.210	29.734
	1.00	12.65						
15	ATOM	833	CA	THR	109	-5.255	-5.257	28.889
	1.00	12.30						
	ATOM	834	CB	THR	109	-5.935	-6.599	29.286
	1.00	14.44						
20	ATOM	835	OG1	THR	109	-5.674	-6.816	30.697
	1.00	15.40						
	ATOM	836	CG2	THR	109	-5.415	-7.780	28.462
	1.00	13.97						
	ATOM	837	C	THR	109	-5.579	-4.839	27.469
	1.00	11.75						
25	ATOM	838	O	THR	109	-6.711	-4.454	27.199
	1.00	12.42						
	ATOM	839	N	SER	110	-4.630	-4.859	26.538
	1.00	11.20						
30	ATOM	840	CA	SER	110	-4.879	-4.532	25.155
	1.00	10.80						
	ATOM	841	CB	SER	110	-4.941	-3.031	24.965
	1.00	10.12						
	ATOM	842	OG	SER	110	-5.204	-2.682	23.632
	1.00	11.48						
35	ATOM	843	C	SER	110	-3.690	-5.105	24.405
	1.00	11.32						
	ATOM	844	O	SER	110	-2.547	-5.207	24.920
	1.00	12.50						
40	ATOM	845	N	ASP	111	-4.042	-5.590	23.213
	1.00	10.79						
	ATOM	846	CA	ASP	111	-3.119	-6.087	22.199
	1.00	12.25						
	ATOM	847	CB	ASP	111	-2.447	-4.890	21.486
	1.00	13.12						
45	ATOM	848	CG	ASP	111	-3.520	-3.986	20.911
	1.00	13.55						
	ATOM	849	OD1	ASP	111	-4.270	-4.400	20.041
	1.00	13.05						
50	ATOM	850	OD2	ASP	111	-3.631	-2.862	21.377
	1.00	14.27						
	ATOM	851	C	ASP	111	-2.044	-7.029	22.706
	1.00	13.33						
	ATOM	852	O	ASP	111	-0.825	-6.910	22.477
	1.00	14.68						
55	ATOM	853	N	GLY	112	-2.491	-7.933	23.566
	1.00	13.67						



	ATOM	854	CA	GLY	112	-1.595	-8.956	24.072
	1.00	10.73						
	ATOM	855	C	GLY	112	-0.959	-8.664	25.418
	1.00	9.91						
5	ATOM	856	O	GLY	112	-0.094	-9.437	25.783
	1.00	9.84						
	ATOM	857	N	SER	113	-1.218	-7.600	26.180
	1.00	9.51						
	ATOM	858	CA	SER	113	-0.518	-7.452	27.424
10	1.00	8.66						
	ATOM	859	CB	SER	113	0.851	-6.812	27.189
	1.00	6.40						
	ATOM	860	OG	SER	113	1.712	-6.818	28.313
	1.00	5.69						
15	ATOM	861	C	SER	113	-1.350	-6.588	28.292
	1.00	8.88						
	ATOM	862	O	SER	113	-2.213	-5.874	27.803
	1.00	11.46						
	ATOM	863	N	VAL	114	-1.190	-6.691	29.594
20	1.00	10.48						
	ATOM	864	CA	VAL	114	-1.787	-5.641	30.395
	1.00	9.89						
	ATOM	865	CB	VAL	114	-2.304	-6.209	31.826
	1.00	11.18						
25	ATOM	866	CG1	VAL	114	-1.870	-7.641	32.032
	1.00	10.85						
	ATOM	867	CG2	VAL	114	-1.853	-5.324	32.981
	1.00	10.22						
	ATOM	868	C	VAL	114	-0.666	-4.581	30.466
30	1.00	10.04						
	ATOM	869	O	VAL	114	0.535	-4.838	30.231
	1.00	9.80						
	ATOM	870	N	TYR	115	-1.145	-3.368	30.683
	1.00	9.29						
35	ATOM	871	CA	TYR	115	-0.390	-2.144	30.797
	1.00	9.53						
	ATOM	872	CB	TYR	115	-0.789	-1.113	29.736
	1.00	8.60						
	ATOM	873	CG	TYR	115	-0.417	-1.372	28.281
40	1.00	8.75						
	ATOM	874	CD1	TYR	115	0.505	-0.554	27.607
	1.00	7.26						
	ATOM	875	CE1	TYR	115	0.788	-0.783	26.275
	1.00	7.31						
45	ATOM	876	CD2	TYR	115	-1.043	-2.408	27.631
	1.00	8.71						
	ATOM	877	CE2	TYR	115	-0.778	-2.646	26.312
	1.00	9.10						
	ATOM	878	CZ	TYR	115	0.126	-1.843	25.640
50	1.00	8.99						
	ATOM	879	OH	TYR	115	0.311	-2.161	24.309
	1.00	9.97						
	ATOM	880	C	TYR	115	-0.747	-1.545	32.151
	1.00	10.03						
55	ATOM	881	O	TYR	115	-1.874	-1.667	32.641
	1.00	10.65						

	ATOM	882	N	ASP	116	0.206	-0.895	32.794
	1.00	10.05						
	ATOM	883	CA	ASP	116	-0.094	-0.187	34.027
	1.00	10.95						
5	ATOM	884	CB	ASP	116	1.092	-0.386	34.982
	1.00	10.88						
	ATOM	885	CG	ASP	116	1.153	-1.800	35.539
	1.00	12.59						
10	ATOM	886	OD1	ASP	116	2.085	-2.539	35.245
	1.00	12.09						
	ATOM	887	OD2	ASP	116	0.281	-2.189	36.298
	1.00	13.31						
	ATOM	888	C	ASP	116	-0.323	1.296	33.610
	1.00	10.73						
15	ATOM	889	O	ASP	116	0.307	1.792	32.656
	1.00	9.98						
	ATOM	890	N	ILE	117	-1.259	1.980	34.272
	1.00	10.31						
	ATOM	891	CA	ILE	117	-1.768	3.320	33.944
20	1.00	11.24						
	ATOM	892	CB	ILE	117	-3.316	3.226	33.891
	1.00	11.80						
	ATOM	893	CG2	ILE	117	-3.969	4.626	33.919
	1.00	12.99						
25	ATOM	894	CG1	ILE	117	-3.714	2.409	32.671
	1.00	11.14						
	ATOM	895	CD1	ILE	117	-5.195	2.011	32.763
	1.00	11.30						
	ATOM	896	C	ILE	117	-1.287	4.285	35.037
30	1.00	11.21						
	ATOM	897	O	ILE	117	-1.484	4.007	36.236
	1.00	11.16						
	ATOM	898	N	TYR	118	-0.646	5.368	34.631
	1.00	9.67						
35	ATOM	899	CA	TYR	118	-0.039	6.351	35.530
	1.00	10.44						
	ATOM	900	CB	TYR	118	1.481	6.226	35.585
	1.00	8.83						
	ATOM	901	CG	TYR	118	1.994	4.842	35.959
40	1.00	9.45						
	ATOM	902	CD1	TYR	118	2.210	3.919	34.944
	1.00	9.25						
	ATOM	903	CE1	TYR	118	2.696	2.663	35.241
	1.00	10.55						
45	ATOM	904	CD2	TYR	118	2.261	4.524	37.284
	1.00	9.83						
	ATOM	905	CE2	TYR	118	2.756	3.269	37.601
	1.00	11.19						
	ATOM	906	CZ	TYR	118	2.969	2.341	36.566
50	1.00	11.73						
	ATOM	907	OH	TYR	118	3.484	1.078	36.857
	1.00	11.26						
	ATOM	908	C	TYR	118	-0.329	7.801	35.103
	1.00	10.46						
55	ATOM	909	O	TYR	118	-0.521	8.073	33.914
	1.00	9.48						

	ATOM	910	N	ARG	119	-0.335	8.724	36.053
	1.00	11.66						
	ATOM	911	CA	ARG	119	-0.553	10.155	35.779
	1.00	14.61						
5	ATOM	912	CB	ARG	119	-1.973	10.621	36.265
	1.00	17.40						
	ATOM	913	CG	ARG	119	-2.089	12.021	36.952
	1.00	23.37						
	ATOM	914	CD	ARG	119	-3.471	12.483	37.490
10	1.00	26.18						
	ATOM	915	NE	ARG	119	-4.356	12.883	36.371
	1.00	30.66						
	ATOM	916	CZ	ARG	119	-5.263	13.922	36.488
	1.00	33.03						
15	ATOM	917	NH1	ARG	119	-5.325	14.574	37.682
	1.00	34.14						
	ATOM	918	NH2	ARG	119	-6.085	14.337	35.453
	1.00	32.49						
	ATOM	919	C	ARG	119	0.546	10.899	36.536
20	1.00	14.29						
	ATOM	920	O	ARG	119	0.866	10.575	37.684
	1.00	12.19						
	ATOM	921	N	THR	120	1.155	11.881	35.873
	1.00	15.13						
25	ATOM	922	CA	THR	120	2.243	12.707	36.395
	1.00	16.87						
	ATOM	923	CB	THR	120	3.620	12.350	35.730
	1.00	19.15						
	ATOM	924	OG1	THR	120	3.353	12.150	34.313
30	1.00	22.72						
	ATOM	925	CG2	THR	120	4.277	11.062	36.276
	1.00	21.25						
	ATOM	926	C	THR	120	1.859	14.152	35.996
	1.00	15.72						
35	ATOM	927	O	THR	120	0.915	14.327	35.236
	1.00	11.42						
	ATOM	928	N	GLN	121	2.510	15.213	36.480
	1.00	18.27						
	ATOM	929	CA	GLN	121	2.180	16.591	36.057
40	1.00	18.87						
	ATOM	930	CB	GLN	121	1.490	17.333	37.150
	1.00	20.46						
	ATOM	931	CG	GLN	121	0.818	18.647	36.686
	1.00	22.49						
45	ATOM	932	CD	GLN	121	0.528	19.470	37.910
	1.00	23.15						
	ATOM	933	OE1	GLN	121	-0.609	19.866	38.201
	1.00	24.23						
	ATOM	934	NE2	GLN	121	1.566	19.744	38.711
50	1.00	25.37						
	ATOM	935	C	GLN	121	3.469	17.311	35.724
	1.00	17.45						
	ATOM	936	O	GLN	121	4.483	17.265	36.429
	1.00	17.70						
55	ATOM	937	N	ARG	122	3.507	17.884	34.557
	1.00	16.86						

	ATOM	938	CA	ARG	122	4.666	18.646	34.205
	1.00	17.38						
	ATOM	939	CB	ARG	122	4.919	18.431	32.738
	1.00	17.17						
5	ATOM	940	CG	ARG	122	4.983	16.936	32.371
	1.00	17.66						
	ATOM	941	CD	ARG	122	6.035	16.268	33.234
	1.00	19.91						
10	ATOM	942	NE	ARG	122	7.405	16.749	33.155
	1.00	20.83						
	ATOM	943	CZ	ARG	122	8.060	17.199	32.061
	1.00	21.20						
	ATOM	944	NH1	ARG	122	7.485	17.275	30.834
	1.00	24.32						
15	ATOM	945	NH2	ARG	122	9.359	17.539	32.223
	1.00	21.52						
	ATOM	946	C	ARG	122	4.285	20.099	34.550
	1.00	18.00						
20	ATOM	947	O	ARG	122	3.127	20.529	34.309
	1.00	15.92						
	ATOM	948	N	VAL	123	5.264	20.778	35.187
	1.00	17.31						
	ATOM	949	CA	VAL	123	5.100	22.174	35.581
	1.00	17.49						
25	ATOM	950	CB	VAL	123	5.204	22.292	37.118
	1.00	18.68						
	ATOM	951	CG1	VAL	123	5.057	23.752	37.578
	1.00	18.13						
30	ATOM	952	CG2	VAL	123	4.025	21.495	37.756
	1.00	17.08						
	ATOM	953	C	VAL	123	6.132	23.037	34.888
	1.00	18.01						
	ATOM	954	O	VAL	123	7.348	22.820	34.956
	1.00	19.01						
35	ATOM	955	N	ASN	124	5.550	23.905	34.058
	1.00	18.77						
	ATOM	956	CA	ASN	124	6.246	24.856	33.204
	1.00	18.46						
40	ATOM	957	CB	ASN	124	6.839	25.978	34.049
	1.00	18.90						
	ATOM	958	CG	ASN	124	5.688	26.871	34.516
	1.00	19.83						
	ATOM	959	OD1	ASN	124	5.841	27.521	35.548
	1.00	21.50						
45	ATOM	960	ND2	ASN	124	4.457	26.916	33.966
	1.00	18.83						
	ATOM	961	C	ASN	124	7.288	24.274	32.301
	1.00	17.97						
50	ATOM	962	O	ASN	124	8.485	24.580	32.249
	1.00	19.21						
	ATOM	963	N	GLN	125	6.718	23.436	31.457
	1.00	17.42						
	ATOM	964	CA	GLN	125	7.513	22.692	30.522
	1.00	15.95						
55	ATOM	965	CB	GLN	125	7.340	21.162	30.781
	1.00	18.71						

	ATOM	966	CG	GLN	125	7.771	20.765	32.189
	1.00	20.97						
	ATOM	967	CD	GLN	125	9.279	20.949	32.484
	1.00	23.57						
5	ATOM	968	OE1	GLN	125	10.114	20.190	31.977
	1.00	24.89						
	ATOM	969	NE2	GLN	125	9.737	21.872	33.335
	1.00	24.87						
10	ATOM	970	C	GLN	125	6.994	23.068	29.153
	1.00	14.36						
	ATOM	971	O	GLN	125	5.828	23.466	28.999
	1.00	13.68						
	ATOM	972	N	PRO	126	7.847	22.921	28.138
	1.00	13.24						
15	ATOM	973	CD	PRO	126	9.304	22.804	28.272
	1.00	13.21						
	ATOM	974	CA	PRO	126	7.444	22.936	26.773
	1.00	11.98						
20	ATOM	975	CB	PRO	126	8.686	22.587	25.972
	1.00	12.53						
	ATOM	976	CG	PRO	126	9.718	22.098	26.983
	1.00	12.93						
	ATOM	977	C	PRO	126	6.291	22.004	26.506
	1.00	11.75						
25	ATOM	978	O	PRO	126	6.115	20.913	27.073
	1.00	11.75						
	ATOM	979	N	SER	127	5.462	22.567	25.667
	1.00	11.03						
	ATOM	980	CA	SER	127	4.315	21.866	25.199
30	1.00	10.71						
	ATOM	981	CB	SER	127	3.081	22.230	26.043
	1.00	10.39						
	ATOM	982	OG	SER	127	2.618	23.555	25.769
	1.00	11.05						
35	ATOM	983	C	SER	127	4.178	22.399	23.787
	1.00	12.20						
	ATOM	984	O	SER	127	4.895	23.295	23.342
	1.00	12.63						
40	ATOM	985	N	ILE	128	3.221	21.771	23.145
	1.00	10.76						
	ATOM	986	CA	ILE	128	2.628	22.112	21.877
	1.00	12.75						
	ATOM	987	CB	ILE	128	1.518	20.968	21.777
	1.00	11.99						
45	ATOM	988	CG2	ILE	128	0.710	20.959	23.097
	1.00	13.03						
	ATOM	989	CG1	ILE	128	0.526	21.141	20.704
	1.00	13.86						
	ATOM	990	CD1	ILE	128	-0.807	20.429	21.073
50	1.00	11.79						
	ATOM	991	C	ILE	128	2.166	23.616	21.786
	1.00	12.49						
	ATOM	992	O	ILE	128	2.010	24.160	20.689
	1.00	11.61						
55	ATOM	993	N	ILE	129	1.911	24.268	22.923
	1.00	11.55						

	ATOM	994	CA	ILE	129	1.335	25.625	23.051
	1.00	12.87						
	ATOM	995	CB	ILE	129	0.050	25.264	23.942
	1.00	12.77						
5	ATOM	996	CG2	ILE	129	0.063	25.810	25.372
	1.00	12.19						
	ATOM	997	CG1	ILE	129	-1.129	25.730	23.208
	1.00	13.88						
10	ATOM	998	CD1	ILE	129	-1.556	24.732	22.166
	1.00	13.59						
	ATOM	999	C	ILE	129	2.414	26.584	23.628
	1.00	12.93						
	ATOM	1000	O	ILE	129	2.195	27.795	23.818
	1.00	15.68						
15	ATOM	1001	N	GLY	130	3.595	26.061	24.001
	1.00	12.43						
	ATOM	1002	CA	GLY	130	4.647	26.814	24.669
	1.00	11.72						
20	ATOM	1003	C	GLY	130	4.752	26.447	26.146
	1.00	10.71						
	ATOM	1004	O	GLY	130	4.105	25.502	26.558
	1.00	11.85						
	ATOM	1005	N	THR	131	5.552	27.094	26.999
	1.00	10.63						
25	ATOM	1006	CA	THR	131	5.633	26.774	28.422
	1.00	10.32						
	ATOM	1007	CB	THR	131	6.507	27.778	29.134
	1.00	10.53						
30	ATOM	1008	OG1	THR	131	7.632	27.883	28.294
	1.00	13.71						
	ATOM	1009	CG2	THR	131	6.969	27.382	30.523
	1.00	9.71						
	ATOM	1010	C	THR	131	4.284	26.743	29.108
	1.00	10.05						
35	ATOM	1011	O	THR	131	3.512	27.720	29.121
	1.00	9.35						
	ATOM	1012	N	ALA	132	4.066	25.560	29.667
	1.00	9.69						
40	ATOM	1013	CA	ALA	132	2.783	25.208	30.228
	1.00	10.33						
	ATOM	1014	CB	ALA	132	1.913	24.574	29.134
	1.00	8.89						
	ATOM	1015	C	ALA	132	2.850	24.229	31.413
	1.00	10.62						
45	ATOM	1016	O	ALA	132	3.926	23.711	31.762
	1.00	11.81						
	ATOM	1017	N	THR	133	1.721	24.123	32.100
	1.00	11.01						
50	ATOM	1018	CA	THR	133	1.541	23.113	33.134
	1.00	12.77						
	ATOM	1019	CB	THR	133	1.145	23.789	34.478
	1.00	13.67						
	ATOM	1020	OG1	THR	133	2.360	24.447	34.897
	1.00	15.23						
55	ATOM	1021	CG2	THR	133	0.651	22.835	35.592
	1.00	13.85						



	ATOM	1022	C	THR	133	0.457	22.171	32.632
	1.00	12.16						
	ATOM	1023	O	THR	133	-0.628	22.577	32.176
	1.00	12.10						
5	ATOM	1024	N	PHE	134	0.737	20.871	32.678
	1.00	12.04						
	ATOM	1025	CA	PHE	134	-0.191	19.880	32.118
	1.00	10.26						
10	ATOM	1026	CB	PHE	134	0.014	19.753	30.593
	1.00	9.74						
	ATOM	1027	CG	PHE	134	1.450	19.497	30.158
	1.00	10.10						
	ATOM	1028	CD1	PHE	134	2.345	20.538	30.021
	1.00	9.16						
15	ATOM	1029	CD2	PHE	134	1.867	18.209	29.908
	1.00	9.83						
	ATOM	1030	CE1	PHE	134	3.652	20.313	29.647
	1.00	10.74						
	ATOM	1031	CE2	PHE	134	3.177	17.977	29.532
20	1.00	10.39						
	ATOM	1032	CZ	PHE	134	4.074	19.013	29.401
	1.00	11.34						
	ATOM	1033	C	PHE	134	0.017	18.520	32.763
	1.00	10.97						
25	ATOM	1034	O	PHE	134	1.072	18.261	33.334
	1.00	9.19						
	ATOM	1035	N	TYR	135	-1.010	17.700	32.729
	1.00	10.76						
	ATOM	1036	CA	TYR	135	-0.896	16.327	33.212
30	1.00	11.10						
	ATOM	1037	CB	TYR	135	-2.247	15.786	33.699
	1.00	11.88						
	ATOM	1038	CG	TYR	135	-2.575	16.298	35.090
	1.00	15.19						
35	ATOM	1039	CD1	TYR	135	-1.816	15.890	36.171
	1.00	17.24						
	ATOM	1040	CE1	TYR	135	-2.054	16.351	37.457
	1.00	17.77						
	ATOM	1041	CD2	TYR	135	-3.607	17.183	35.298
40	1.00	17.57						
	ATOM	1042	CE2	TYR	135	-3.862	17.655	36.594
	1.00	18.71						
	ATOM	1043	CZ	TYR	135	-3.082	17.237	37.661
	1.00	18.40						
45	ATOM	1044	OH	TYR	135	-3.300	17.720	38.949
	1.00	21.11						
	ATOM	1045	C	TYR	135	-0.420	15.448	32.070
	1.00	11.69						
	ATOM	1046	O	TYR	135	-0.785	15.621	30.892
50	1.00	9.54						
	ATOM	1047	N	GLN	136	0.343	14.419	32.467
	1.00	10.85						
	ATOM	1048	CA	GLN	136	0.927	13.498	31.514
	1.00	10.50						
55	ATOM	1049	CB	GLN	136	2.404	13.687	31.779
	1.00	10.66						

	ATOM	1050	CG	GLN	136	3.383	13.299	30.739
	1.00	11.87						
	ATOM	1051	CD	GLN	136	4.796	13.457	31.286
	1.00	12.64						
5	ATOM	1052	OE1	GLN	136	5.081	13.041	32.405
	1.00	14.21						
	ATOM	1053	NE2	GLN	136	5.779	13.990	30.586
	1.00	13.11						
10	ATOM	1054	C	GLN	136	0.324	12.109	31.805
	1.00	10.27						
	ATOM	1055	O	GLN	136	0.386	11.631	32.935
	1.00	8.17						
	ATOM	1056	N	TYR	137	-0.377	11.467	30.878
	1.00	11.70						
15	ATOM	1057	CA	TYR	137	-0.971	10.159	31.163
	1.00	12.76						
	ATOM	1058	CB	TYR	137	-2.397	10.001	30.623
	1.00	15.14						
20	ATOM	1059	CG	TYR	137	-3.416	11.066	30.980
	1.00	17.31						
	ATOM	1060	CD1	TYR	137	-3.310	11.813	32.136
	1.00	20.43						
	ATOM	1061	CE1	TYR	137	-4.280	12.773	32.443
	1.00	22.42						
25	ATOM	1062	CD2	TYR	137	-4.483	11.262	30.111
	1.00	20.69						
	ATOM	1063	CE2	TYR	137	-5.460	12.203	30.402
	1.00	22.72						
30	ATOM	1064	CZ	TYR	137	-5.354	12.951	31.583
	1.00	23.68						
	ATOM	1065	OH	TYR	137	-6.404	13.809	31.984
	1.00	26.30						
	ATOM	1066	C	TYR	137	-0.113	9.085	30.487
	1.00	13.36						
35	ATOM	1067	O	TYR	137	0.402	9.271	29.361
	1.00	14.35						
	ATOM	1068	N	TRP	138	0.043	7.923	31.137
	1.00	11.84						
40	ATOM	1069	CA	TRP	138	0.942	6.879	30.640
	1.00	8.71						
	ATOM	1070	CB	TRP	138	2.273	6.810	31.444
	1.00	8.01						
	ATOM	1071	CG	TRP	138	3.238	8.005	31.558
	1.00	8.31						
45	ATOM	1072	CD2	TRP	138	4.474	8.150	30.977
	1.00	7.73						
	ATOM	1073	CE2	TRP	138	4.909	9.361	31.532
	1.00	8.67						
50	ATOM	1074	CE3	TRP	138	5.287	7.474	30.094
	1.00	7.01						
	ATOM	1075	CD1	TRP	138	2.949	9.072	32.391
	1.00	9.63						
	ATOM	1076	NE1	TRP	138	3.986	9.872	32.348
	1.00	9.33						
55	ATOM	1077	CZ2	TRP	138	6.134	9.919	31.237
	1.00	7.84						

	ATOM	1078	CZ3	TRP	138	6.516	8.026	29.791
	1.00	9.01						
	ATOM	1079	CH2	TRP	138	6.935	9.224	30.349
	1.00	8.58						
5	ATOM	1080	C	TRP	138	0.270	5.502	30.768
	1.00	9.46						
	ATOM	1081	O	TRP	138	-0.484	5.232	31.709
	1.00	8.88						
10	ATOM	1082	N	SER	139	0.417	4.664	29.751
	1.00	11.22						
	ATOM	1083	CA	SER	139	0.116	3.213	29.806
	1.00	11.52						
	ATOM	1084	CB	SER	139	-0.762	2.735	28.692
	1.00	11.35						
15	ATOM	1085	OG	SER	139	-2.138	2.978	28.917
	1.00	13.26						
	ATOM	1086	C	SER	139	1.477	2.565	29.547
	1.00	10.74						
	ATOM	1087	O	SER	139	2.063	2.824	28.486
	1.00	11.43						
20	ATOM	1088	N	VAL	140	2.027	1.780	30.460
	1.00	9.74						
	ATOM	1089	CA	VAL	140	3.306	1.139	30.256
	1.00	9.29						
25	ATOM	1090	CB	VAL	140	4.191	1.381	31.514
	1.00	9.45						
	ATOM	1091	CG1	VAL	140	5.580	0.791	31.315
	1.00	9.67						
30	ATOM	1092	CG2	VAL	140	4.329	2.918	31.750
	1.00	9.25						
	ATOM	1093	C	VAL	140	3.057	-0.352	30.005
	1.00	9.37						
	ATOM	1094	O	VAL	140	2.461	-1.081	30.830
	1.00	8.14						
35	ATOM	1095	N	ARG	141	3.521	-0.782	28.835
	1.00	10.69						
	ATOM	1096	CA	ARG	141	3.404	-2.199	28.443
	1.00	11.96						
	ATOM	1097	CB	ARG	141	3.757	-2.391	26.945
	1.00	11.92						
40	ATOM	1098	CG	ARG	141	3.431	-3.843	26.522
	1.00	12.57						
	ATOM	1099	CD	ARG	141	3.684	-4.280	25.085
	1.00	11.72						
45	ATOM	1100	NE	ARG	141	2.351	-4.384	24.581
	1.00	15.48						
	ATOM	1101	CZ	ARG	141	1.620	-5.350	24.013
	1.00	13.58						
	ATOM	1102	NH1	ARG	141	1.970	-6.616	23.698
	1.00	12.83						
50	ATOM	1103	NH2	ARG	141	0.361	-4.935	23.852
	1.00	13.32						
	ATOM	1104	C	ARG	141	4.314	-3.116	29.302
	1.00	9.52						
55	ATOM	1105	O	ARG	141	5.544	-2.998	29.343
	1.00	8.68						

	ATOM	1106	N	ARG	142	3.671	-4.076	30.002
	1.00	10.19						
	ATOM	1107	CA	ARG	142	4.421	-5.006	30.855
	1.00	10.06						
5	ATOM	1108	CB	ARG	142	3.456	-5.843	31.649
	1.00	9.21						
	ATOM	1109	CG	ARG	142	2.846	-5.061	32.777
	1.00	9.22						
10	ATOM	1110	CD	ARG	142	2.254	-5.997	33.780
	1.00	8.97						
	ATOM	1111	NE	ARG	142	1.440	-5.256	34.689
	1.00	8.70						
	ATOM	1112	CZ	ARG	142	0.517	-5.842	35.463
	1.00	9.47						
15	ATOM	1113	NH1	ARG	142	0.338	-7.202	35.422
	1.00	9.32						
	ATOM	1114	NH2	ARG	142	-0.249	-5.019	36.194
	1.00	9.02						
20	ATOM	1115	C	ARG	142	5.337	-5.888	30.030
	1.00	9.64						
	ATOM	1116	O	ARG	142	6.540	-5.988	30.280
	1.00	11.41						
	ATOM	1117	N	ASN	143	4.786	-6.349	28.929
	1.00	9.44						
25	ATOM	1118	CA	ASN	143	5.490	-7.214	27.997
	1.00	11.07						
	ATOM	1119	CB	ASN	143	4.523	-8.194	27.420
	1.00	15.18						
30	ATOM	1120	CG	ASN	143	4.798	-9.487	28.077
	1.00	19.83						
	ATOM	1121	OD1	ASN	143	4.354	-9.693	29.224
	1.00	21.43						
	ATOM	1122	ND2	ASN	143	5.589	-10.295	27.336
	1.00	21.58						
35	ATOM	1123	C	ASN	143	6.111	-6.441	26.874
	1.00	9.46						
	ATOM	1124	O	ASN	143	5.418	-6.281	25.886
	1.00	7.69						
40	ATOM	1125	N	HIS	144	7.379	-6.024	26.936
	1.00	8.08						
	ATOM	1126	CA	HIS	144	7.902	-5.078	25.959
	1.00	8.77						
	ATOM	1127	CB	HIS	144	9.257	-4.577	26.418
	1.00	9.04						
45	ATOM	1128	CG	HIS	144	9.304	-3.876	27.793
	1.00	10.00						
	ATOM	1129	CD2	HIS	144	10.469	-3.373	28.345
	1.00	9.60						
50	ATOM	1130	ND1	HIS	144	8.353	-3.647	28.706
	1.00	12.26						
	ATOM	1131	CE1	HIS	144	8.904	-3.055	29.762
	1.00	10.72						
	ATOM	1132	NE2	HIS	144	10.191	-2.893	29.533
	1.00	9.65						
55	ATOM	1133	C	HIS	144	8.017	-5.649	24.551
	1.00	11.38						



	ATOM	1134	O	HIS	144	8.203	-6.861	24.375
	1.00	10.85						
	ATOM	1135	N	ARG	145	7.844	-4.832	23.505
	1.00	10.56						
5	ATOM	1136	CA	ARG	145	7.940	-5.277	22.118
	1.00	9.42						
	ATOM	1137	CB	ARG	145	6.587	-5.753	21.574
	1.00	8.54						
	ATOM	1138	CG	ARG	145	5.436	-4.936	22.132
10	1.00	9.46						
	ATOM	1139	CD	ARG	145	4.240	-4.414	21.384
	1.00	10.47						
	ATOM	1140	NE	ARG	145	3.196	-5.305	20.989
	1.00	8.83						
15	ATOM	1141	CZ	ARG	145	1.931	-4.970	20.643
	1.00	8.35						
	ATOM	1142	NH1	ARG	145	1.339	-3.775	20.631
	1.00	7.40						
	ATOM	1143	NH2	ARG	145	1.255	-5.917	20.002
20	1.00	9.04						
	ATOM	1144	C	ARG	145	8.377	-4.136	21.243
	1.00	9.13						
	ATOM	1145	O	ARG	145	8.135	-2.979	21.592
	1.00	10.52						
25	ATOM	1146	N	SER	146	8.954	-4.467	20.093
	1.00	8.90						
	ATOM	1147	CA	SER	146	9.332	-3.505	19.086
	1.00	9.55						
	ATOM	1148	CB	SER	146	10.781	-3.760	18.716
30	1.00	8.66						
	ATOM	1149	OG	SER	146	11.646	-3.526	19.809
	1.00	10.90						
	ATOM	1150	C	SER	146	8.452	-3.487	17.826
	1.00	9.89						
35	ATOM	1151	O	SER	146	8.698	-2.675	16.921
	1.00	11.00						
	ATOM	1152	N	SER	147	7.456	-4.366	17.671
	1.00	9.25						
	ATOM	1153	CA	SER	147	6.519	-4.300	16.562
40	1.00	10.93						
	ATOM	1154	CB	SER	147	7.027	-5.161	15.395
	1.00	13.60						
	ATOM	1155	OG	SER	147	7.396	-6.472	15.843
	1.00	17.36						
45	ATOM	1156	C	SER	147	5.134	-4.781	16.995
	1.00	10.10						
	ATOM	1157	O	SER	147	5.045	-5.529	17.975
	1.00	11.84						
	ATOM	1158	N	GLY	148	4.025	-4.387	16.384
50	1.00	9.36						
	ATOM	1159	CA	GLY	148	2.718	-4.855	16.790
	1.00	8.24						
	ATOM	1160	C	GLY	148	1.658	-3.894	16.327
	1.00	8.56						
55	ATOM	1161	O	GLY	148	1.885	-3.108	15.405
	1.00	10.71						

	ATOM	1162	N	SER	149	0.482	-3.983	16.909
	1.00	9.40						
	ATOM	1163	CA	SER	149	-0.602	-3.056	16.648
	1.00	10.95						
5	ATOM	1164	CB	SER	149	-1.780	-3.739	16.037
	1.00	12.62						
	ATOM	1165	OG	SER	149	-1.203	-4.402	14.925
	1.00	20.18						
10	ATOM	1166	C	SER	149	-1.039	-2.529	18.002
	1.00	11.07						
	ATOM	1167	O	SER	149	-0.827	-3.223	19.016
	1.00	10.99						
	ATOM	1168	N	VAL	150	-1.551	-1.292	18.042
	1.00	10.64						
15	ATOM	1169	CA	VAL	150	-2.081	-0.728	19.273
	1.00	10.28						
	ATOM	1170	CB	VAL	150	-1.224	0.457	19.813
	1.00	10.28						
20	ATOM	1171	CG1	VAL	150	-1.893	1.108	20.981
	1.00	8.88						
	ATOM	1172	CG2	VAL	150	0.152	-0.067	20.216
	1.00	10.04						
	ATOM	1173	C	VAL	150	-3.475	-0.217	18.919
	1.00	11.39						
25	ATOM	1174	O	VAL	150	-3.657	0.510	17.936
	1.00	11.90						
	ATOM	1175	N	ASN	151	-4.456	-0.661	19.661
	1.00	11.61						
30	ATOM	1176	CA	ASN	151	-5.782	-0.144	19.539
	1.00	13.38						
	ATOM	1177	CB	ASN	151	-6.745	-1.312	19.809
	1.00	15.35						
	ATOM	1178	CG	ASN	151	-8.191	-0.831	19.729
	1.00	19.10						
35	ATOM	1179	OD1	ASN	151	-8.500	0.361	19.505
	1.00	21.76						
	ATOM	1180	ND2	ASN	151	-9.156	-1.690	20.022
	1.00	19.23						
40	ATOM	1181	C	ASN	151	-5.885	1.011	20.561
	1.00	13.32						
	ATOM	1182	O	ASN	151	-6.102	0.814	21.778
	1.00	13.06						
	ATOM	1183	N	THR	152	-5.744	2.285	20.109
	1.00	12.70						
45	ATOM	1184	CA	THR	152	-5.670	3.429	21.041
	1.00	10.80						
	ATOM	1185	CB	THR	152	-5.402	4.741	20.273
	1.00	9.08						
50	ATOM	1186	OG1	THR	152	-6.506	5.026	19.423
	1.00	9.66						
	ATOM	1187	CG2	THR	152	-4.107	4.646	19.511
	1.00	8.63						
	ATOM	1188	C	THR	152	-6.908	3.610	21.922
	1.00	12.10						
55	ATOM	1189	O	THR	152	-6.824	3.983	23.109
	1.00	12.41						

	ATOM	1190	N	ALA	153	-8.062	3.223	21.362
	1.00	12.52						
	ATOM	1191	CA	ALA	153	-9.365	3.291	22.021
	1.00	13.18						
5	ATOM	1192	CB	ALA	153	-10.422	2.571	21.212
	1.00	14.11						
	ATOM	1193	C	ALA	153	-9.390	2.663	23.410
	1.00	13.55						
10	ATOM	1194	O	ALA	153	-9.868	3.237	24.389
	1.00	11.50						
	ATOM	1195	N	ASN	154	-8.688	1.526	23.512
	1.00	13.78						
	ATOM	1196	CA	ASN	154	-8.642	0.814	24.781
	1.00	13.58						
15	ATOM	1197	CB	ASN	154	-7.924	-0.499	24.613
	1.00	14.46						
	ATOM	1198	CG	ASN	154	-8.774	-1.450	23.787
	1.00	15.29						
20	ATOM	1199	OD1	ASN	154	-8.242	-2.299	23.070
	1.00	16.38						
	ATOM	1200	ND2	ASN	154	-10.098	-1.363	23.743
	1.00	15.71						
	ATOM	1201	C	ASN	154	-7.982	1.583	25.887
	1.00	13.14						
25	ATOM	1202	O	ASN	154	-8.449	1.613	27.026
	1.00	12.59						
	ATOM	1203	N	HIS	155	-6.889	2.234	25.498
	1.00	12.89						
30	ATOM	1204	CA	HIS	155	-6.134	3.043	26.440
	1.00	13.28						
	ATOM	1205	CB	HIS	155	-4.802	3.434	25.858
	1.00	12.80						
	ATOM	1206	CG	HIS	155	-3.934	2.210	25.718
	1.00	11.42						
35	ATOM	1207	CD2	HIS	155	-3.836	1.416	24.591
	1.00	10.81						
	ATOM	1208	ND1	HIS	155	-3.200	1.700	26.674
	1.00	9.77						
40	ATOM	1209	CE1	HIS	155	-2.651	0.622	26.199
	1.00	9.97						
	ATOM	1210	NE2	HIS	155	-3.033	0.454	24.962
	1.00	11.54						
	ATOM	1211	C	HIS	155	-6.908	4.318	26.755
	1.00	13.91						
45	ATOM	1212	O	HIS	155	-7.062	4.658	27.932
	1.00	14.83						
	ATOM	1213	N	PHE	156	-7.439	5.021	25.752
	1.00	14.01						
50	ATOM	1214	CA	PHE	156	-8.141	6.257	26.072
	1.00	14.84						
	ATOM	1215	CB	PHE	156	-8.592	6.997	24.827
	1.00	14.21						
	ATOM	1216	CG	PHE	156	-7.473	7.369	23.896
	1.00	14.75						
55	ATOM	1217	CD1	PHE	156	-6.201	7.640	24.371
	1.00	16.50						

	ATOM	1218	CD2	PHE	156	-7.723	7.428	22.544
	1.00	15.81						
	ATOM	1219	CE1	PHE	156	-5.187	7.970	23.480
	1.00	16.11						
5	ATOM	1220	CE2	PHE	156	-6.705	7.762	21.658
	1.00	15.84						
	ATOM	1221	CZ	PHE	156	-5.435	8.039	22.124
	1.00	15.88						
10	ATOM	1222	C	PHE	156	-9.382	5.954	26.906
	1.00	15.07						
	ATOM	1223	O	PHE	156	-9.769	6.777	27.733
	1.00	14.39						
	ATOM	1224	N	ASN	157	-9.998	4.775	26.741
	1.00	15.95						
15	ATOM	1225	CA	ASN	157	-11.188	4.463	27.487
	1.00	16.78						
	ATOM	1226	CB	ASN	157	-11.947	3.247	26.911
	1.00	19.91						
20	ATOM	1227	CG	ASN	157	-12.692	3.666	25.658
	1.00	21.97						
	ATOM	1228	OD1	ASN	157	-12.844	2.871	24.723
	1.00	23.02						
	ATOM	1229	ND2	ASN	157	-13.152	4.918	25.484
	1.00	22.77						
25	ATOM	1230	C	ASN	157	-10.865	4.175	28.900
	1.00	16.15						
	ATOM	1231	O	ASN	157	-11.579	4.674	29.773
	1.00	16.04						
30	ATOM	1232	N	ALA	158	-9.781	3.426	29.138
	1.00	16.31						
	ATOM	1233	CA	ALA	158	-9.319	3.129	30.494
	1.00	15.97						
	ATOM	1234	CB	ALA	158	-8.057	2.270	30.451
	1.00	16.14						
35	ATOM	1235	C	ALA	158	-8.968	4.411	31.265
	1.00	15.64						
	ATOM	1236	O	ALA	158	-9.334	4.645	32.446
	1.00	15.58						
40	ATOM	1237	N	TRP	159	-8.223	5.257	30.544
	1.00	15.76						
	ATOM	1238	CA	TRP	159	-7.821	6.552	31.114
	1.00	15.15						
	ATOM	1239	CB	TRP	159	-6.966	7.314	30.077
	1.00	14.73						
45	ATOM	1240	CG	TRP	159	-5.581	6.715	29.752
	1.00	15.51						
	ATOM	1241	CD2	TRP	159	-4.763	7.058	28.689
	1.00	15.24						
50	ATOM	1242	CE2	TRP	159	-3.698	6.146	28.818
	1.00	15.37						
	ATOM	1243	CE3	TRP	159	-4.769	7.967	27.653
	1.00	14.42						
	ATOM	1244	CD1	TRP	159	-5.023	5.673	30.479
	1.00	16.38						
55	ATOM	1245	NE1	TRP	159	-3.886	5.350	29.897
	1.00	14.73						

	ATOM	1246	CZ2	TRP	159	-2.648	6.129	27.922
	1.00	12.93						
	ATOM	1247	CZ3	TRP	159	-3.718	7.949	26.765
	1.00	14.15						
5	ATOM	1248	CH2	TRP	159	-2.678	7.043	26.901
	1.00	14.30						
	ATOM	1249	C	TRP	159	-9.063	7.367	31.526
	1.00	14.08						
10	ATOM	1250	O	TRP	159	-9.173	7.852	32.677
	1.00	13.42						
	ATOM	1251	N	ALA	160	-10.062	7.392	30.651
	1.00	13.53						
	ATOM	1252	CA	ALA	160	-11.307	8.092	30.906
	1.00	15.69						
15	ATOM	1253	CB	ALA	160	-12.248	7.868	29.726
	1.00	16.17						
	ATOM	1254	C	ALA	160	-12.001	7.663	32.188
	1.00	17.30						
20	ATOM	1255	O	ALA	160	-12.385	8.505	33.015
	1.00	16.76						
	ATOM	1256	N	SER	161	-12.076	6.354	32.474
	1.00	19.40						
	ATOM	1257	CA	SER	161	-12.799	5.887	33.642
	1.00	21.24						
25	ATOM	1258	CB	SER	161	-13.287	4.489	33.431
	1.00	21.88						
	ATOM	1259	OG	SER	161	-12.407	3.847	32.515
	1.00	24.44						
30	ATOM	1260	C	SER	161	-11.964	5.918	34.877
	1.00	21.71						
	ATOM	1261	O	SER	161	-12.392	5.514	35.946
	1.00	24.49						
	ATOM	1262	N	HIS	162	-10.712	6.282	34.759
	1.00	23.09						
35	ATOM	1263	CA	HIS	162	-9.899	6.476	35.932
	1.00	24.28						
	ATOM	1264	CB	HIS	162	-8.462	5.957	35.756
	1.00	26.20						
40	ATOM	1265	CG	HIS	162	-8.372	4.525	36.263
	1.00	27.93						
	ATOM	1266	CD2	HIS	162	-8.372	3.431	35.418
	1.00	29.19						
	ATOM	1267	ND1	HIS	162	-8.356	4.063	37.523
	1.00	27.81						
45	ATOM	1268	CE1	HIS	162	-8.362	2.734	37.460
	1.00	29.60						
	ATOM	1269	NE2	HIS	162	-8.366	2.358	36.196
	1.00	30.08						
50	ATOM	1270	C	HIS	162	-9.870	7.965	36.145
	1.00	24.43						
	ATOM	1271	O	HIS	162	-9.187	8.427	37.059
	1.00	25.01						
	ATOM	1272	N	GLY	163	-10.594	8.702	35.302
	1.00	24.39						
55	ATOM	1273	CA	GLY	163	-10.836	10.108	35.509
	1.00	24.50						

	ATOM	1274	C	GLY	163	-9.860	10.930	34.735
	1.00	26.12						
	ATOM	1275	O	GLY	163	-9.693	12.118	35.003
	1.00	27.42						
5	ATOM	1276	N	LEU	164	-9.231	10.416	33.695
	1.00	26.82						
	ATOM	1277	CA	LEU	164	-8.277	11.191	32.910
	1.00	27.23						
10	ATOM	1278	CB	LEU	164	-7.044	10.365	32.732
	1.00	28.71						
	ATOM	1279	CG	LEU	164	-5.870	10.394	33.748
	1.00	28.96						
	ATOM	1280	CD1	LEU	164	-6.313	10.578	35.218
	1.00	29.11						
15	ATOM	1281	CD2	LEU	164	-5.109	9.096	33.505
	1.00	29.11						
	ATOM	1282	C	LEU	164	-8.824	11.631	31.569
	1.00	27.74						
20	ATOM	1283	O	LEU	164	-8.570	11.052	30.519
	1.00	27.52						
	ATOM	1284	N	THR	165	-9.577	12.737	31.598
	1.00	29.28						
	ATOM	1285	CA	THR	165	-10.232	13.318	30.432
	1.00	29.12						
25	ATOM	1286	CB	THR	165	-11.074	14.530	30.985
	1.00	30.69						
	ATOM	1287	OG1	THR	165	-11.760	15.097	29.861
	1.00	31.47						
30	ATOM	1288	CG2	THR	165	-10.227	15.686	31.634
	1.00	30.40						
	ATOM	1289	C	THR	165	-9.218	13.719	29.337
	1.00	28.99						
	ATOM	1290	O	THR	165	-8.017	13.858	29.623
	1.00	29.54						
35	ATOM	1291	N	LEU	166	-9.641	13.898	28.072
	1.00	27.70						
	ATOM	1292	CA	LEU	166	-8.746	14.319	26.983
	1.00	27.24						
40	ATOM	1293	CB	LEU	166	-8.422	13.284	25.835
	1.00	27.12						
	ATOM	1294	CG	LEU	166	-7.481	12.109	26.084
	1.00	27.81						
	ATOM	1295	CD1	LEU	166	-7.435	11.307	24.774
	1.00	28.93						
45	ATOM	1296	CD2	LEU	166	-6.070	12.560	26.494
	1.00	27.08						
	ATOM	1297	C	LEU	166	-9.593	15.334	26.271
	1.00	25.11						
50	ATOM	1298	O	LEU	166	-10.797	15.041	26.120
	1.00	24.48						
	ATOM	1299	N	GLY	167	-8.932	16.364	25.727
	1.00	23.38						
	ATOM	1300	CA	GLY	167	-9.610	17.412	24.968
	1.00	21.60						
55	ATOM	1301	C	GLY	167	-9.629	17.078	23.482
	1.00	21.20						

	ATOM	1302	O	GLY	167	-9.760	15.889	23.095
	1.00	22.34						
	ATOM	1303	N	THR	168	-9.432	18.098	22.645
	1.00	19.20						
5	ATOM	1304	CA	THR	168	-9.390	17.997	21.191
	1.00	17.79						
	ATOM	1305	CB	THR	168	-9.760	19.453	20.735
	1.00	19.15						
10	ATOM	1306	OG1	THR	168	-10.323	19.282	19.441
	1.00	21.89						
	ATOM	1307	CG2	THR	168	-8.613	20.458	20.690
	1.00	18.08						
	ATOM	1308	C	THR	168	-7.986	17.461	20.832
	1.00	15.71						
15	ATOM	1309	O	THR	168	-6.987	17.903	21.384
	1.00	14.65						
	ATOM	1310	N	MET	169	-7.843	16.481	19.953
	1.00	14.44						
20	ATOM	1311	CA	MET	169	-6.576	15.814	19.662
	1.00	14.83						
	ATOM	1312	CB	MET	169	-6.836	14.483	18.935
	1.00	15.04						
	ATOM	1313	CG	MET	169	-7.727	13.517	19.684
	1.00	16.43						
25	ATOM	1314	SD	MET	169	-7.005	13.060	21.275
	1.00	20.33						
	ATOM	1315	CE	MET	169	-6.344	11.447	20.893
	1.00	18.80						
30	ATOM	1316	C	MET	169	-5.637	16.648	18.797
	1.00	14.85						
	ATOM	1317	O	MET	169	-6.024	17.252	17.775
	1.00	17.21						
	ATOM	1318	N	ASP	170	-4.409	16.773	19.220
	1.00	13.83						
35	ATOM	1319	CA	ASP	170	-3.401	17.330	18.307
	1.00	13.73						
	ATOM	1320	C	ASP	170	-2.670	16.197	17.581
	1.00	10.96						
40	ATOM	1321	O	ASP	170	-3.383	15.283	17.156
	1.00	12.91						
	ATOM	1322	CB	ASP	170	-2.365	18.025	18.072
	1.00	14.89						
	ATOM	1323	CG	ASP	170	-1.803	19.443	18.160
	1.00	17.35						
45	ATOM	1324	OD1	ASP	170	-2.595	20.457	18.060
	1.00	20.00						
	ATOM	1325	OD2	ASP	170	-0.538	19.626	18.333
	1.00	20.00						
50	ATOM	1326	N	TYR	171	-1.371	16.150	17.418
	1.00	10.61						
	ATOM	1327	CA	TYR	171	-0.722	15.072	16.692
	1.00	11.47						
	ATOM	1328	CB	TYR	171	0.658	15.560	16.280
	1.00	10.30						
55	ATOM	1329	CG	TYR	171	1.776	15.763	17.280
	1.00	10.95						

	ATOM	1330	CD1	TYR	171	2.416	14.672	17.876
	1.00	11.20						
	ATOM	1331	CE1	TYR	171	3.502	14.868	18.710
	1.00	11.22						
5	ATOM	1332	CD2	TYR	171	2.214	17.053	17.525
	1.00	10.25						
	ATOM	1333	CE2	TYR	171	3.298	17.256	18.365
	1.00	11.78						
10	ATOM	1334	CZ	TYR	171	3.942	16.171	18.954
	1.00	10.98						
	ATOM	1335	OH	TYR	171	5.018	16.389	19.792
	1.00	9.29						
	ATOM	1336	C	TYR	171	-0.664	13.748	17.485
	1.00	11.01						
15	ATOM	1337	O	TYR	171	-0.816	13.794	18.713
	1.00	10.53						
	ATOM	1338	N	GLN	172	-0.495	12.610	16.787
	1.00	10.87						
20	ATOM	1339	CA	GLN	172	-0.503	11.246	17.332
	1.00	9.53						
	ATOM	1340	CB	GLN	172	-1.889	10.738	17.176
	1.00	10.18						
	ATOM	1341	CG	GLN	172	-2.244	9.357	17.630
	1.00	9.79						
25	ATOM	1342	CD	GLN	172	-3.732	9.052	17.489
	1.00	9.76						
	ATOM	1343	OE1	GLN	172	-4.267	8.939	16.379
	1.00	10.99						
30	ATOM	1344	NE2	GLN	172	-4.460	8.919	18.599
	1.00	9.74						
	ATOM	1345	C	GLN	172	0.492	10.523	16.436
	1.00	8.72						
	ATOM	1346	O	GLN	172	0.248	10.353	15.235
	1.00	9.11						
35	ATOM	1347	N	ILE	173	1.605	10.159	17.064
	1.00	6.96						
	ATOM	1348	CA	ILE	173	2.851	9.711	16.474
	1.00	6.99						
40	ATOM	1349	CB	ILE	173	3.719	11.020	16.654
	1.00	9.21						
	ATOM	1350	CG2	ILE	173	4.913	11.022	17.588
	1.00	8.02						
	ATOM	1351	CG1	ILE	173	4.058	11.318	15.266
	1.00	10.65						
45	ATOM	1352	CD1	ILE	173	2.845	12.113	14.728
	1.00	11.75						
	ATOM	1353	C	ILE	173	3.439	8.426	17.059
	1.00	5.19						
50	ATOM	1354	O	ILE	173	3.197	8.136	18.232
	1.00	5.97						
	ATOM	1355	N	VAL	174	4.168	7.610	16.319
	1.00	5.30						
	ATOM	1356	CA	VAL	174	4.915	6.536	16.939
	1.00	5.81						
55	ATOM	1357	CB	VAL	174	5.054	5.263	16.052
	1.00	5.74						

	ATOM	1358	CG1	VAL	174	6.070	4.324	16.682
	1.00	6.61						
	ATOM	1359	CG2	VAL	174	3.714	4.576	15.922
	1.00	4.99						
5	ATOM	1360	C	VAL	174	6.265	7.190	17.103
	1.00	4.60						
	ATOM	1361	O	VAL	174	6.897	7.637	16.138
	1.00	6.58						
10	ATOM	1362	N	ALA	175	6.711	7.294	18.342
	1.00	6.06						
	ATOM	1363	CA	ALA	175	7.916	8.061	18.607
	1.00	4.93						
	ATOM	1364	CB	ALA	175	7.557	9.318	19.381
	1.00	6.89						
15	ATOM	1365	C	ALA	175	9.029	7.410	19.367
	1.00	3.97						
	ATOM	1366	O	ALA	175	8.739	6.644	20.319
	1.00	8.33						
20	ATOM	1367	N	VAL	176	10.275	7.682	18.999
	1.00	3.82						
	ATOM	1368	CA	VAL	176	11.309	7.278	19.902
	1.00	6.89						
	ATOM	1369	CB	VAL	176	12.544	6.510	19.224
	1.00	9.34						
25	ATOM	1370	CG1	VAL	176	11.996	5.545	18.180
	1.00	7.08						
	ATOM	1371	CG2	VAL	176	13.562	7.396	18.645
	1.00	10.56						
30	ATOM	1372	C	VAL	176	11.770	8.574	20.585
	1.00	8.28						
	ATOM	1373	O	VAL	176	11.913	9.639	19.970
	1.00	7.87						
	ATOM	1374	N	GLU	177	11.846	8.510	21.912
	1.00	9.10						
35	ATOM	1375	CA	GLU	177	12.231	9.635	22.760
	1.00	8.39						
	ATOM	1376	CB	GLU	177	11.195	9.842	23.821
	1.00	8.89						
40	ATOM	1377	CG	GLU	177	11.585	10.946	24.816
	1.00	10.47						
	ATOM	1378	CD	GLU	177	10.463	11.616	25.586
	1.00	12.55						
	ATOM	1379	OE1	GLU	177	10.780	12.349	26.527
	1.00	14.06						
45	ATOM	1380	OE2	GLU	177	9.286	11.451	25.259
	1.00	11.52						
	ATOM	1381	C	GLU	177	13.517	9.156	23.393
	1.00	9.30						
50	ATOM	1382	O	GLU	177	13.565	7.957	23.766
	1.00	10.91						
	ATOM	1383	N	GLY	178	14.506	10.044	23.506
	1.00	7.47						
	ATOM	1384	CA	GLY	178	15.748	9.766	24.177
	1.00	6.20						
55	ATOM	1385	C	GLY	178	16.025	10.868	25.187
	1.00	8.83						

	ATOM	1386	O	GLY	178	15.621	12.042	25.010
	1.00	8.10						
	ATOM	1387	N	TYR	179	16.693	10.485	26.273
	1.00	7.84						
5	ATOM	1388	CA	TYR	179	17.120	11.392	27.288
	1.00	8.12						
	ATOM	1389	CB	TYR	179	16.265	11.279	28.515
	1.00	8.58						
10	ATOM	1390	CG	TYR	179	16.568	12.436	29.468
	1.00	12.04						
	ATOM	1391	CD1	TYR	179	17.399	12.215	30.546
	1.00	12.92						
	ATOM	1392	CE1	TYR	179	17.723	13.240	31.395
	1.00	14.76						
15	ATOM	1393	CD2	TYR	179	16.046	13.693	29.239
	1.00	12.66						
	ATOM	1394	CE2	TYR	179	16.363	14.734	30.096
	1.00	14.65						
	ATOM	1395	CZ	TYR	179	17.202	14.485	31.159
20	1.00	15.49						
	ATOM	1396	OH	TYR	179	17.565	15.497	32.006
	1.00	18.12						
	ATOM	1397	C	TYR	179	18.550	11.061	27.639
	1.00	9.22						
25	ATOM	1398	O	TYR	179	18.855	10.147	28.414
	1.00	10.38						
	ATOM	1399	N	PHE	180	19.425	11.865	27.019
	1.00	8.36						
	ATOM	1400	CA	PHE	180	20.844	11.857	27.265
30	1.00	9.15						
	ATOM	1401	CB	PHE	180	21.070	12.542	28.622
	1.00	9.13						
	ATOM	1402	CG	PHE	180	20.877	14.060	28.563
	1.00	9.20						
35	ATOM	1403	CD1	PHE	180	19.621	14.613	28.705
	1.00	9.46						
	ATOM	1404	CD2	PHE	180	21.983	14.868	28.362
	1.00	11.38						
	ATOM	1405	CE1	PHE	180	19.455	15.988	28.651
40	1.00	10.39						
	ATOM	1406	CE2	PHE	180	21.829	16.257	28.304
	1.00	10.50						
	ATOM	1407	CZ	PHE	180	20.563	16.793	28.449
	1.00	10.79						
45	ATOM	1408	C	PHE	180	21.464	10.460	27.223
	1.00	10.10						
	ATOM	1409	O	PHE	180	22.029	9.956	28.189
	1.00	10.49						
	ATOM	1410	N	SER	181	21.345	9.832	26.067
50	1.00	12.63						
	ATOM	1411	CA	SER	181	21.791	8.442	25.903
	1.00	11.89						
	ATOM	1412	CB	SER	181	20.605	7.545	26.290
	1.00	10.63						
55	ATOM	1413	OG	SER	181	19.481	7.785	25.454
	1.00	9.90						

	ATOM	1414	C	SER	181	22.261	8.187	24.458
	1.00	11.07						
	ATOM	1415	O	SER	181	22.630	9.127	23.718
	1.00	10.95						
5	ATOM	1416	N	SER	182	22.284	6.908	24.101
	1.00	8.87						
	ATOM	1417	CA	SER	182	22.600	6.513	22.769
	1.00	9.70						
10	ATOM	1418	CB	SER	182	24.021	6.016	22.725
	1.00	8.44						
	ATOM	1419	OG	SER	182	24.934	7.051	23.106
	1.00	11.70						
	ATOM	1420	C	SER	182	21.630	5.414	22.351
	1.00	8.32						
15	ATOM	1421	O	SER	182	20.985	4.798	23.214
	1.00	8.91						
	ATOM	1422	N	GLY	183	21.467	5.216	21.045
	1.00	8.19						
20	ATOM	1423	CA	GLY	183	20.679	4.114	20.539
	1.00	9.01						
	ATOM	1424	C	GLY	183	20.553	4.164	19.022
	1.00	11.09						
	ATOM	1425	O	GLY	183	21.209	4.956	18.319
	1.00	11.68						
25	ATOM	1426	N	SER	184	19.610	3.365	18.544
	1.00	11.79						
	ATOM	1427	CA	SER	184	19.353	3.151	17.133
	1.00	11.40						
30	ATOM	1428	CB	SER	184	20.242	2.035	16.632
	1.00	11.41						
	ATOM	1429	OG	SER	184	20.580	2.124	15.275
	1.00	15.69						
	ATOM	1430	C	SER	184	17.911	2.693	17.021
	1.00	10.12						
35	ATOM	1431	O	SER	184	17.446	1.896	17.852
	1.00	11.52						
	ATOM	1432	N	ALA	185	17.201	3.136	16.005
	1.00	8.63						
40	ATOM	1433	CA	ALA	185	15.890	2.616	15.747
	1.00	6.71						
	ATOM	1434	CB	ALA	185	14.812	3.279	16.605
	1.00	5.28						
	ATOM	1435	C	ALA	185	15.548	2.893	14.307
	1.00	8.30						
45	ATOM	1436	O	ALA	185	15.852	3.971	13.757
	1.00	8.44						
	ATOM	1437	N	SER	186	14.890	1.908	13.712
	1.00	8.21						
50	ATOM	1438	CA	SER	186	14.334	2.079	12.414
	1.00	7.45						
	ATOM	1439	CB	SER	186	15.201	1.275	11.479
	1.00	8.66						
	ATOM	1440	OG	SER	186	14.672	1.319	10.175
	1.00	8.84						
55	ATOM	1441	C	SER	186	12.886	1.622	12.514
	1.00	9.02						

	ATOM	1442	O	SER	186	12.620	0.477	12.885
	1.00	7.60						
	ATOM	1443	N	ILE	187	11.875	2.493	12.354
	1.00	8.36						
5	ATOM	1444	CA	ILE	187	10.517	2.013	12.471
	1.00	9.26						
	ATOM	1445	CB	ILE	187	9.933	2.345	13.963
	1.00	12.57						
10	ATOM	1446	CG2	ILE	187	11.001	2.794	14.977
	1.00	10.66						
	ATOM	1447	CG1	ILE	187	8.893	3.361	13.908
	1.00	11.46						
	ATOM	1448	CD1	ILE	187	7.616	2.580	14.124
	1.00	12.68						
15	ATOM	1449	C	ILE	187	9.623	2.516	11.337
	1.00	9.78						
	ATOM	1450	O	ILE	187	9.873	3.551	10.672
	1.00	10.18						
20	ATOM	1451	N	THR	188	8.595	1.714	11.054
	1.00	7.46						
	ATOM	1452	CA	THR	188	7.617	2.008	10.005
	1.00	8.18						
	ATOM	1453	CB	THR	188	7.753	0.972	8.796
	1.00	6.41						
25	ATOM	1454	OG1	THR	188	9.078	1.119	8.291
	1.00	5.82						
	ATOM	1455	CG2	THR	188	6.704	1.165	7.675
	1.00	5.98						
30	ATOM	1456	C	THR	188	6.218	1.951	10.610
	1.00	6.88						
	ATOM	1457	O	THR	188	5.864	1.006	11.312
	1.00	7.67						
	ATOM	1458	N	VAL	189	5.464	2.989	10.331
	1.00	7.06						
35	ATOM	1459	CA	VAL	189	4.104	3.196	10.803
	1.00	9.10						
	ATOM	1460	CB	VAL	189	3.913	4.657	11.335
	1.00	9.32						
40	ATOM	1461	CG1	VAL	189	2.554	4.764	11.989
	1.00	9.82						
	ATOM	1462	CG2	VAL	189	4.969	5.015	12.359
	1.00	7.64						
	ATOM	1463	C	VAL	189	3.135	2.976	9.664
	1.00	8.74						
45	ATOM	1464	O	VAL	189	3.432	3.326	8.514
	1.00	9.63						
	ATOM	1465	N	SER	190	1.967	2.498	10.032
	1.00	10.99						
50	ATOM	1466	CA	SER	190	0.853	2.346	9.138
	1.00	13.10						
	ATOM	1467	CB	SER	190	0.966	1.065	8.258
	1.00	15.33						
	ATOM	1468	OG	SER	190	1.169	-0.182	8.908
	1.00	15.84						
55	ATOM	1469	C	SER	190	-0.415	2.271	9.950
	1.00	14.43						

ATOM	1470	O	SER	190	-1.439	2.580	9.354
	1.00						17.68
ATOM	1471	OXT	SER	190	-0.392	1.975	11.150
	1.00						12.62

5

10 A portion of the three-dimensional crystal
 structure of a mutant of the *B. circulans* xylanase containing
 an intramolecular disulfide bond is shown in Figure 4. In
 this mutant serine 100 and asparagine 148 have been mutated
 to cysteine. The disulfide which is formed links the last
 strand of sheet III to the alpha-helix. The structure of
 15 this mutant is identical to the wild-type enzyme except for
 the side chains of residues 100 and 148 and some very minor
 shifts of nearby atoms. The same region of the
 superimposed structures of the *B. circulans* and *T. harzianum*
 xylanases is shown in Figure 5. Further details of the
 analyses will be provided in the examples, however, one can
 see that although there are some sequence differences
 20 between the *B. circulans* and *T. harzianum* xylanases near the site
 of the manufactured disulfide and some small position
 differences at other nearby residues, the structure of the
T. harzianum xylanase is virtually identical to the structure
 of the *B. circulans* xylanase at the positions of the
 mutations. The sequence alignment (Figure 1) shows that
 25 the sequence homology of the various xylanases in the
 vicinity of residues 98 to 100 and 148 to 152 is very good.
 One would therefore expect that the structures of other
 related xylanases would be similar enough that they could
 be modified with the introduction of an intramolecular
 30 disulfide bond linking sheet III to the alpha-helix and
 that this disulfide bond would stabilize them in a similar
 manner as taught in the present invention.

35 Similarly one would expect that sequence changes
 made at the N-terminal end of the *B. circulans* xylanase, which
 produced a more stable xylanase, could be made at
 corresponding positions in other family G xylanases, with
 a reasonable expectation of success. For example, the

strategy to substitute the Asn residue N-8 of *B. circulans* xylanase by Tyr and Phe to yield more stable mutants, can be readily applied to fungal xylanases of *A. niger* var. *awamori*, *A. tubigensis* A and *T. ressei* I. These fungal xylanases, like the bacterial *B. circulans* xylanase, possesses the same target Asn residue, available for the same mutation.

For some xylanases with reduced sequence homology to the *B. circulans* xylanase it may be necessary to make other mutations to increase the homology in the vicinity of the introduced intramolecular disulfide bond or N-terminal mutation. In other words it may be necessary to make another xylanase more like the *B. circulans* xylanase before the disulfide bond could be formed successfully or before a useful N-terminal mutation is made. Throughout the application reference is made to amino acid positions based on the *B. circulans* xylanase, as a reference. Figure 1 is provided in order to determine the corresponding position in other family G xylanases.

In the modification of family G xylanases, the *B. circulans* xylanase (BCX) was chosen to exemplify the principles of the present invention. This enzyme is only moderately thermostable at temperatures up to 55°C. For application of this enzyme in pretreatment of kraft-pulp to enhance bleaching, a higher temperature stability is desirable. As noted previously, a xylanase which has a higher pH optimum, would also be beneficial in the bleaching step. Such a modified enzyme would also be useful in the food industry.

As noted previously, the chief application of the modified xylanase is for pulp biobleaching in the production of paper. Before bleaching process, the pulp is hot at a temperature range of 55-70°C and in an alkaline

state. Many commercial wild-type xylanases (*T. reesei* and *B. pumilus*) only function at 55°C and some require acidic pH. Therefore the desirable improvements in a mutant xylanase are higher functional temperature (temperature optimum) and pH (pH optimum), with the former characteristic as the most important. Xylanase of higher temperature optimum can be used to treat pulp at high temperature without idle period of cooling. With higher functional pH (pH optimal), the mutant enzyme would require less or no acid to neutralize the pulp which is basic at that stage. The economic benefits include saving in time, acid for neutralization and no acidic corrosion of the equipments. Therefore a desirable xylanase mutant would have a temperature optimum approaching 70°C and a pH optimum approaching 9 in pulp bleaching. Of course any measurable improvement over the wild type xylanase, BCX (54°C, pH 7) would be beneficial.

In the parent application (U.S. Serial No. 08/044,621), the improvement of mutant was measured in terms of thermostability, ie, its ability to survive incubation at high temperature in buffer without any substrate. Increased thermostability means an increase of 2°C to 15°C, while maintaining at least 60% of activity, compared to wild type xylanase, after incubation at an elevated temperature. Such a pursuit of improved thermostability or passive heat-resistance was the sole objective in another publication involving xylanase (Arase et al, 1993). Although this characteristic may be useful and possibly related to the shelf-life of the enzyme, it is not a reliable indicator of the ability of the enzyme to function at that temperature. At the elevated temperature, the enzyme molecule may have been deactivated or unfolded but managed to be quickly refolded or reactivated before assayed at 40°C. Therefore the gain in thermostability or heat-resistance ($T_{1/2}$) does not guarantee that the enzyme remains intact or can function at higher temperature.

An alternative assay was used to determine if the mutant enzyme can function at high temperature. Instead of incubation in buffer without xylan, xylanase is incubated in the same manner with xylan in the buffer. The modified process is designed to evaluate the hydrolysis of soluble xylan by the mutant enzyme at different temperatures. The reducing sugar released was then determined by the HBAH reagent. With addition of xylan in the mixture, the protocol remained essentially the same. The temperature optimum is defined as the highest temperature at which 150% relative enzymatic activity was maintained as compared to performance at 40°C.

A further measure of increased stability, according to the present invention, is an increase in pH optimum in the hydrolysis of xylan. In the present invention, pH optimum has been defined as the highest pH at which the enzyme still maintains 50% of the maximal activity.

In addition to the assay based on the direct hydrolysis of xylan, the mutant xylanases were also tested for their ability to bleach pulp. The temperature optimum and pH optimum in pulp bleaching are defined as the highest temperature and pH at which the brightness gain by the treated pulp was not less than 0.4.

In one aspect of the present invention, the starting point was the solution of the three-dimensional structure of the enzyme (Figure 2). By inspection of the structure, a prediction of the residues, which could be mutated to cysteine, and which would possibly oxidize to form an intra-molecular SS bridge was made. This was accomplished by searching for pairs of residues for which the inter-C-alpha distance was less than 6.6 Å and the inter-C-beta distance was less than 4.5 Å. If either member of the pair was a glycine this pair was ignored

5 because glycines are important for the backbone conformation. Some candidates were excluded because they were involved in the active site of the enzyme. In addition the distance algorithm had selected pairs of residues which were too close, as they were on adjacent strands of one of the beta sheets.

10 Two areas for the introduction of a cysteine residue were selected. These areas are the beta-sheet III and the alpha-helix. Although the alpha-helix itself ranges from amino acids 147 to 155, some residues on either side could potentially be used to form intra-molecular disulfide linkages. Accordingly, the amino acids in the alpha-helix ranging from 143 to 158 and the amino acids on 15 the beta-sheet III ranging from 95 to 109 are potential sites for the introduction of cysteine residues for the formation of an intra-molecular disulphide bond between these two areas. Two pairs of residues were found (details will be provided in the Examples) and the corresponding 20 mutants were constructed, and in both cases the intra-molecular SS bond formed spontaneously.

25 In addition to the intra-molecular SS bond mutant, a second type of disulfide mutant was constructed by joining two protein molecules with an inter-molecular SS bond. For the production of this type of disulfide bond, a cysteine is introduced in each of the two xylanase protein molecules such that the cysteine is on the exterior of the molecule, thus the two molecules can be joined by an 30 inter-molecular disulphide bond. Potential sites of interest include amino acid 15 to 31 of the beta-sheet I; amino acid 43 to 61 of the beta-sheet I; amino acid 87 to 104 of the loop and beta-sheet III; amino acid 133 to 163 of the alpha-helix and surrounding loops; and amino acids 35 177 to 185 of the beta-sheet I.

A third type of mutant unrelated to SS bond formation has also been found to confer stability. These mutants were generated by specific mutagenesis of amino acids at the N-terminus of the xylanase molecule. In one embodiment of the present invention, amino acids 1 to 25 of the xylanase protein are selected for specific mutagenesis. As discussed above, the amino acid numbering is based on the *B. circulans* xylanase. Corresponding amino acids from other family G xylanases can be determined by making reference to Figure 1.

In one example of the present invention, the introduction of tyrosine or phenylalanine by substitution resulted in mutants with increased thermostability, temperature optimum and pH optimum, when compared to the wild type protein. In another embodiment of the present invention, the introduction of proline at amino acid position 22, by substitution resulted in a more stable mutant. In a further example of the present invention, the stability of the mutant could be increased by combining two or mutations in a single molecule. In some examples the effect of two or more mutants was additive and in other examples the effect was co-operative.

The selected amino acids referred to above are based on the amino acid sequence of the *B. circulans* xylanase sequence. The present invention is not limited to producing a thermostable xylanase from this bacterial source, but includes the production of a thermostable xylanase for other sources, as listed in Table 1 for example. The choice of suitable amino acids to target for mutagenesis in xylanases from other sources will be obvious to those skilled in the art by comparing the sequences and choosing the amino acids corresponding to those identified for the *B. circulans* xylanase.

The present invention will be further illustrated by way of the following examples, which are not to be construed as limiting. In these examples the xylanase mutants, which were constructed, are summarized in Table 2.

5

Table 2
Xylanase Mutants

Name	Mutation	Type of Mutation
TS1	S100C N148C	intra-molecular SS bond
TS2	V98C A152C	intra-molecular SS bond
TS3a	D4Y N8F	N-terminal Mutation
TS3	S100C N148C D4Y N8F	intra-molecular SS bond + N-terminal
TS4a	S179C dimer	inter-molecular SS bond
TS4	S100C N148C S179C monomer/dimer mix	intra- + inter-molecular SS bond
TS4M	S100C N148C S179C monomer	intra-molecular SS bond
TS4D	S100C N148C S179C dimer	intra- + inter-molecular SS bond
TS5a	N8Y	N-terminal mutation
TS6a	T3G D4Y N8Y	N-terminal mutation

EXAMPLE 1

CONSTRUCTION OF THE MUTANT TS1

The gene encoding the *B. subtilis* xylanase (see Figure 6), is identical to the *B. circulans* xylanase except at position 147, where a serine (BSX) rather than threonine (BCX) is encoded, (Yang et al, 1988, Nucleic Acid Research 16:7187 and Paice et al, 1986, Archives of Microbiology 144:201-206; all references incorporated herein by reference). The xylanase gene encoded by pBSX was mutated by the uracil containing DNA (UDNA) method (Kunkle et al, 1987, Methods in Enzymology, 154:367-382, which is incorporated herein by reference) to produce the mutant S100C. The coding sequence for this mutant gene was then removed from the vector using PCR. The 5' portion of the resulting PCR product (codons 1-103) was combined with a synthetic gene fragment from the *B. circulans* gene (codons 104-185) to produce the plasmid pCWBCX::S100C. The region containing codons 136-153 of pCWBCX::S100C was replaced with synthetic oligonucleotides to introduce the second cysteine codon at position 148 (N148C). The resultant plasmid contained the S100C and N148C mutations and was called TS1.

All liquid cultures in this and other Examples were grown in either 2YT medium (16 g yeast extract, 10 g bacto-tryptone, 5 g NaCl, 1 L of H₂O), or TB medium (24 g yeast extract, 12 g bacto-tryptone, 10 ml 1 M potassium phosphate buffer pH 7.5, 5 ml of 80% glycerol, 1 L H₂O). The antibiotic ampicillin was added at 150 µg/ml to all cultures of plasmid containing strains. The cultures were grown with shaking at 30°C for protein and plasmid production, and 37°C for the production of single stranded DNA containing particles.

Basic recombinant DNA methods like plasmid DNA isolation, restriction enzyme digestions, the purification of DNA fragments for cloning, ligations, transformations and DNA sequencing were performed as recommended by the enzyme supplier, or the manufacturer of the kit used for

the particular procedure. Polyacrylamide gel electrophoresis of proteins was performed as recommended in the technical literature supplied by Bio-Rad laboratories, Mississauga Ont. Restriction and DNA modification enzymes were purchased from New England Biolabs LTD., Mississauga Ont. Prep-A-Gene DNA purification matrix was purchased from Bio-Rad laboratories, Mississauga Ont. Sequenase, a DNA sequencing kit, was purchased from US Biochemicals, Cleveland Ohio. Oligonucleotide 3' end labelling was performed with a kit from Boehringer Mannheim Canada, Laval PQ. Protein concentration was determined from the molar extinction coefficient of the xylanase: $81,790 \text{ L.mol}^{-1}$.

A 2 ml culture of *Escherichia coli* RZ1032 (HfrKL16PO/45 [lysA(61-62)], dut1, ung1, thi1, relA1, Zbd-279::Tn10, supE44) harbouring pBSX was grown at 37°C with vigorous shaking until the A_{600} reached 0.5, at which time 10 μl of the helper phage, M13KO7, (titre $1 \times 10^{12}/\text{ml}$), was added. After 1 h, 0.5 ml of the culture was subcultured into 20 ml of fresh media containing 50 μg kanamycin/ml, and 100 μg ampicillin/ml. This culture was shaken at 200 rpm for 16 h at 37°C. The supernatant containing the single stranded DNA containing particles (SSDNAP) was collected after centrifugation of the culture at 4°C for 20 min. at 7000 x g. The SSDNAP were precipitated by the addition of 1/4 volume of 15% PEG-8000/ 14.6% NaCl. After 30 min. at room temperature the precipitate was collected by centrifugation at 7000 x g for 20 min. The precipitate was resuspended in 0.5 ml TE buffer (10mM Tris - HCl, 1 mM EDTA, pH 8), and left on ice for 30 min. Any insoluble material was removed by a brief centrifugation in a microcentrifuge. The supernatant was made up to 1% acetic acid and the resultant precipitate was collected on a 1 cm glass fibre filter by suction filtration. Protein was removed from the precipitated SSDNAP'S, and the DNA bound to the filter by washing the filter under vacuum, with 2 ml of 4 M NaClO₄ in TE buffer. Excess NaClO₄ was removed by

washing the filter with 2 ml of ice cold 70% ethanol. The filter was allowed to air dry for 5 min. at room temperature. The filter was placed into a 500 μ l microcentrifuge tube with a hole in the bottom. This tube was placed inside a 1.5 ml microcentrifuge tube. The single stranded DNA was eluted by the addition of 50 μ l of 0.1X TE buffer to the filter and after 5 min centrifuging the two tubes to recover the liquid in the larger tube. The elution step was repeated. The single stranded DNA was quantified by analysis on agarose gel electrophoresis.

Oligonucleotides were synthesized using an Applied Biosystems model 380B DNA synthesizer. Synthetic oligonucleotides were purified by polyacrylamide gel electrophoresis (PAGE) in 15% gels containing 7 M urea. Oligonucleotides were detected by UV shadowing, cut out and eluted from the gel slices in 1 ml of 0.5 M ammonium acetate, 10 mM magnesium acetate. The oligonucleotides were desalted by passage through a Sep-Pak C18 reverse phase cartridge (Atkinson and Smith, 1984, In: Oligonucleotide synthesis a practical approach. Gait, N. J., editor. IRL press, Washington). The oligonucleotides were eluted with 20 % acetonitrile, and the concentration was determined by reading the A_{260} of the solution. For the production of S100C the following oligonucleotide was synthesized:

SEQ ID NO:4

Codons 96 97 98 99 100 101 102 103 104

5'- GGT ACT GTA AAA TGT GAT GGG GGT ACA - 3'

The oligonucleotide was phosphorylated for use in mutagenesis. 100 to 200 pmol of the oligonucleotide was mixed with 2 μ l of 10X kinase buffer (500 mM Tris-HCl, pH 7.6, 100 mM $MgCl_2$, 100 mM dithiothreitol (DTT), 1.0 mM spermidine, 10 mM adenosine triphosphate (ATP)), and the volume was adjusted with water to a final volume of 20 μ l.

The reaction was initiated by the addition of 10U of T4 polynucleotide kinase. The reaction was performed at 37°C for 1 h, after which the reaction was terminated by heating at 70°C for 10 min. Oligonucleotides prepared in this fashion were ready for use in the UDNA mutagenesis method.

The phosphorylated mutagenic oligonucleotide primer (20 pmol, 2 μ l), was mixed with the ssUDNA (0.5 pmol, 7 μ l); 1 μ l of 10X DNA synthesis buffer (200 mM Tris-HCl, pH 7.5, 100 mM MgCl₂, 500 mM NaCl, 10 mM DTT). The DNA's were annealed by heating the mixture to 70°C, and then slowly cooled to room temperature. The mutagenesis reaction was then performed by the addition of 10 μ l of the DNA synthesis mixture (1 μ l 10X synthesis buffer (200 mM Tris-HCl, pH 7.5, 100 mM MgCl₂, 100 mM DTT), 1 μ l 5 mM deoxynucleotide triphosphates (dNTPs), 1 μ l 10 mM ATP, 6 μ l H₂O, 1 μ l, 5U, T4 DNA ligase, 0.25 μ l, 2.5U, T7 DNA polymerase). The reaction mixture was kept on ice for 5 min, then at room temperature for 5 min., and finally incubated at 37°C for 60 to 90 min. The reaction was terminated by the addition of 3 μ l 50 mM EDTA. The reaction products were analyzed by standard agarose gel electrophoresis (Sambrook et al, 1989, Molecular cloning: A laboratory manual, 2nd edition). A 5 μ l portion of this mixture was used to transform the *E. coli* strain MV1190 (deletion (lac-proAB), thi, supE44, deletion (srl-recA)306::Tn10(tet') [F':traD36, proAB, lacI⁴deletion M15]) or BHM 71-18 (deletion (lac-proAB), thi, supE44, [mutS::Tn10(tet')]).

After transformation the bacteria were plated onto solid media (2YT) containing 150 μ g ampicillin/ml. Individual colonies were picked and transferred to a fresh plate in a grid pattern of 100 colonies per plate. After overnight growth at 37°C, the colonies were transferred to Hybond-N nylon filter membranes (Amersham, Canada, Oakville Ont.), the colonies were lysed, and the DNA fixed to these

filters by well established procedures (Sambrook et al, 1989, Molecular cloning: a laboratory manual).

Oligonucleotide probes were synthesized using a 3' end labelling kit from Boehringer Mannheim. 100 pmol of oligonucleotide were dissolved in 4 μ l H₂O. The reaction mixture was completed as follows: 4 μ l of 5X tailing buffer (1M potassium cacodylate, 0.125 M Tris-HCl, bovine serum albumin (BSA) 1.25 mg/ml, pH 6.6), 4 μ l 25 mM CoCl₂, 1 μ l 1 mM digoxigenin-dideoxy-uracil triphosphate (DIG-ddUTP), 6 μ l H₂O, 1 μ l terminal transferase (50U). The mixture was reacted at 37°C for 15 min., then 2 μ l of glycogen was added (0.2 μ g / μ l in 0.2 M EDTA). The labelled oligonucleotide was precipitated by the addition of 2.5 μ l of 4 M LiCl, and 75 μ l of ice cold, -20°C, 95% ethanol. After 2 h at - 20°C the precipitate was collected by centrifugation at 12,000 g for 30 min. The pellet was washed with 100 μ l ice cold 70% ethanol, and then air dried in a fume hood.

The filters containing the colonies were washed free of cell debris in 2X SSC (SSC buffer is 0.15 M NaCl, 0.015 M sodium citrate, pH 7.0), 0.1% SDS, by gently rubbing the surface of the filter with a wet tissue. After removal of the cell debris, the filters were pre-hybridized in hybridization buffer (5X SSC, 0.1% SDS, 0.02% N-laurylsarkosine, 1% blocking reagent, a commercial product from Boehringer Mannheim), for at least 5 h. After the pre-hybridization, the DIG-labelled oligonucleotide was dissolved in 100 μ l H₂O, and added to 7 ml of hybridization buffer. The hybridization buffer-DIG labelled oligonucleotide mixture was poured onto the filter and the hybridization was then performed in plastic petri dishes at 37°C, with shaking overnight. Excess (unbound) probe was removed by washing the filters twice for 10 min, each time, with 2X SSC, 0.1% SDS at room temperature. Non-specifically

bound probe was removed by washing the filters at 40°C with 0.5 X SSC, 0.1% SDS, again twice for 10 min each time.

5 The filters were then washed in 25 ml of M buffer
(0.1 M maleic acid, 0.15 M NaCl, pH adjusted to 7.5 with
concentrated NaOH). The filter was then incubated in 20 ml
M buffer containing 1% blocking reagent for 30 min. at room
temperature. The solution was then discarded and then
10 further incubated with 10 ml of fresh M buffer with 1%
blocking reagent and 750 mU of anti-DIG-alkaline
phosphatase-conjugate antibody. After 30 min., the filter
was washed with 3 x 20 ml washes of M buffer with 0.3%
Tween 20. The filter was then equilibrated in alkaline
phosphatase buffer (0.1 M Tris-HCl, 0.1 M NaCl, 0.05 M
15 MgCl₂, pH 9.5). The filter was then dipped in a solution of
Lumi-phos, a chemiluminescent alkaline phosphatase
substrate (Boehringer Mannheim). The filter was sealed
into a plastic bag, and incubated at 37°C for 30 min. The
filter in the bag was then exposed to x-ray film for 5 to
20 60 min. Positive colonies were further characterized by
DNA sequencing. The clone chosen for subsequent work
contained plasmid pBSXS100C.

25 Removal of the mature coding sequence of the *B.*
subtilis xylanase gene from its leader sequence was
accomplished using PCR with specific primers. The primers
were designed so that the resulting amplification product
would contain a new NdeI restriction site to allow the
precise fusion of the coding region to the transcriptional
30 signals present in pCWori+. An XbaI site was introduced at
the 3' end to facilitate cloning into pCWori+.

35 The plasmid pBSXS100C was digested with EcoRI to
linearize it, and then it was used as a template for PCR.
The amplification reaction contained, 15 µl of template DNA
(50 ng), 5 µl of 10X buffer (100 mM KCl, 100 mM ammonium
sulfate, 200 mM Tris-HCl pH 8.8, 40 mM magnesium sulfate,

1% Triton X100, 100 μ g/ml BSA), 5 μ l of 5 mM dNTPs, 2.5 μ l 5' primer solution (25 pmol), 2.5 μ l 3' primer solution (25 pmol), 19 μ l H₂O, 1 μ l (1U) Vent DNA polymerase (New England Biolabs). The 5' and 3' primers are shown below:

SEQ ID NO:5

NdeI site

5' BSYSL GC CTG CAG CAT ATG GCT AGC ACA GAC TAC TGG CAA AAT TGG A

SEQ ID NO:6

XbaI site

3' BSXYL GC AAG CTT TCT AGA CTT TAA CCA TTA CTA ACG ATT TTA ATA ATC

The reaction was covered with 50 μ l of paraffin oil to prevent evaporation. The reaction mixture was prewarmed to 94°C without enzyme for 5 min., then the reaction mixture was cooled to 72°C, then the enzyme was added. The reaction was incubated in a temperature cycler for 30 cycles of 94°C 1 min., 55°C 2 min., 72°C for 2 min. The yield of amplification product was approximately 1 μ g of a 700 bp fragment. This fragment was purified from an agarose gel.

The resulting PCR product had an introduced NdeI site at the 5' end to provide a start codon for the xylanase gene when cloned into pCWori+. The xylanase gene was cloned into pCWori+ in two steps. First the 3' portion, codons 105 -185 (Figure 6) was inserted as a 330 bp NdeI - XbaI fragment. This fragment was generated by digesting 200 ng of the PCR product with NdeI and XbaI, and then was purified from an agarose gel. 50 ng of this fragment was ligated with 50 ng of NdeI - XbaI digested and gel purified pCWori+. The clone, pCW3', was identified by hybridization using a probe made by random priming labelling (Sambrook et al, 1989, Molecular cloning: a laboratory manual), with DIG-dUTP, of 50 ng of the PCR product. The second step was to digest the PCR product with NdeI to generate a 318 bp fragment which encodes codons 1 - 104. After gel electrophoresis and

purification, 50 ng of this fragment was ligated to 50 ng of NdeI digested pCW3'. The clones containing a functional xylanase gene were identified by screening transformants on plates containing remazo-brilliant blue xylan (RBBX). Those colonies which made halos, were expressing the gene for xylanase (Kluepfel, 1988, Methods in Enzymology, 154:367-382, which is incorporated herein by reference). This clone was called pCWBSX::S100C.

A version of the *B. circulans* xylanase gene was synthesized to aid in subsequent mutagenesis studies, using the first 103 codons of the natural gene, and 82 codons derived from synthetic DNA fragments (pCWBCX3'SYN, Figure 7). The synthetic gene portion is identical to the natural gene except codons were used, which reflect the frequency of usage for specific amino acid residues in the genes of *E. coli*. The 103 codon portion was replaced with the equivalent portion from pCWBSX::S100C, by isolating the NheI-NdeI restriction fragment of pCWBSX::S100C and ligating it to NheI-NdeI digested pCWBCX3'SYN. After ligation, the mixture was transformed into *E. coli* MV1190. Clones were analyzed by DNA sequencing to verify they carried the S100C mutation. The resultant plasmid was called pCWBCX::S100C.

The plasmid pCWBCX::S100C was purified and digested with the restriction enzymes EagI and NsiI to remove the portion encoding codons 136 to 153. The large plasmid fragment was isolated from an agarose gel as described above. A set of synthetic oligonucleotides: Xyl146C TOP (SEQ ID NO:7); Xyl147C BOTTOM (SEQ ID NO:8) and Xyl148C BOTTOM (SEQ ID NO:9) (as shown below) was synthesized to replace the EagI to NsiI fragment these oligonucleotides encoded the mutations at F146C, T147C, and N148C.

EagI

NsiI

137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152
 GG CCG ACT GGT TCG AAC GCC ACC ATC ACT TGC ACT AAC CAT GTC AAT GCA Xy146C TOP
 C TGA CCA AGC TTG CGG TGG TAG TGA AAG ACA TTG GTA CAG TT Xy147C BOTTOM
 C TGA CCA AGC TTG CGG TGG TAG TGA AAG TGA ACG GTA CAG TT Xy148C BOTTOM

5

10

15

20

For the construction of restriction fragments for cassette mutagenesis, after kinase treatment, complementary oligonucleotides were mixed together (20 pmol of each oligonucleotide), and the mixture was heated to 80°C for 10 min. The mixture was then allowed to slowly cool to room temperature. Portions from the annealed oligonucleotide mixture were then used directly in ligation reactions with the previously digested and purified pCWBCX::S100C. After ligation and transformation, clones carrying the modified EagI-NsiI fragment were identified by hybridization with a DIG-ddUTP labelled oligonucleotide. Once hybridization positive colonies were identified, plasmid DNA was isolated and *E. coli* was re-transformed, to ensure the purity of the clone. DNA sequencing was performed to verify changes at the desired codons.

25

EXAMPLE 2

CONSTRUCTION OF THE MUTANT TS2

30

The plasmid pCWBCX3'SYN was used to transform *E. coli* RZ1032, and single stranded UDNA was prepared as previously described in Example 1. Two mutagenic oligonucleotides for making V98C, and A152C (see below) were used in an *in vitro* DNA synthesis reaction as described in Example 1.

SEQ ID NO:10

Codons 101 100 99 98 97 96 95 94

pCH V98C 5' C ATC ACT TTT GCA AGT ACC TTT ATA 3'

5

SEQ ID NO:11

Codons 155 154 153 152 151 150 149

pCH A152C 5' GGA TTT CCA GCA ATT CAC GTG 3'

10 After transformation, colonies were screened for hybridization to both mutagenic oligonucleotides. The xylanase gene from a hybridization positive clone, TS2, was completely sequenced to ensure only the desired mutations were present.

15

EXAMPLE 3

CONSTRUCTION OF THE MUTANT TS4

20 An additional thermostable mutant containing an inter-molecular disulfide bridge was constructed by a mutation at amino acid position 179 to change the amino acid from a serine to a cysteine (S179C). This mutant was constructed using cassette mutagenesis to make TS4a using the oligonucleotides: S179C-1 (SEQ ID NO:12); S179C-2 (SEQ
25 ID NO:13) and S179C-3 (SEQ ID NO:14) shown below:

Codons 178 179 180 181 182 183 184 185

S179C-1 5' CT GGA TCG TCC AAT GTG ACA GTG TGG TAA AGA TCT TGA

S179C-2 3' TCG AGA CCT ACG AGG TTA CAC

30

S179C-3 3' TGT CAC ACC ATT TCT AGA ACT

35 The plasmid pCWBCX3'SYN was digested with SacI and HindIII. The large fragment was purified from an agarose gel. The oligonucleotides for S179C were processed as described in Example 1, for cassette mutagenesis. This protein contained a single active thiol, however the protein dimerizes spontaneously. It forms a mixture based on the amount of free sulfhydryl from Ellmans reagent testing, and from purification of both the monomer and
40 dim r from the mixture. This mutation was then combined

with TS1, by standard subcloning to produce a mutant called TS4. The mutant TS4M is the combined TS1 + S179C monomeric species and the TS4D is the dimeric species of this mutant. The purity of the monomeric and dimeric species used in the thermostability assays is shown in Figure 8.

EXAMPLE 4

CONSTRUCTION OF MUTATIONS AT THE N-TERMINUS OF *B. CIRCULANS* XYLANASE

Several mutant xylanases with mutations in the N-terminal region, have been constructed via the method of cassette mutagenesis. These mutants are either single, double or triple amino acid changes at positions 3, 4 or 8. All of the gene constructions involved ligations of 2 pairs of oligonucleotides which contained the mutations, into the NheI/BspEI linearized plasmid pXYbc (Figure 9), via the well established recombinant procedures of (i) phosphorylation of the oligonucleotides, (ii) their ligation with the linearized plasmid, (iii) transformation into the *E. coli* competent cells, (iv) identification of the mutant transformants via hybridization with the labelled oligonucleotide as probe, and (v) confirmation of the mutation through gene sequencing. These procedures have been fully described in the preceding Examples. The oligonucleotides used for the production of various N-terminus mutants are shown below.

(1) TS5a mutant, where the asparagine-8 (N-8) has been converted into tyrosine (Y).

The oligonucleotides for the cassette mutagenesis are XY8Y-1 (SEQ ID NO:15), XY8Y-2 (SEQ ID NO:16), XY-11-2

(SEQ ID NO:17) and XY-16-1 (SEQ ID NO:18), and are as show below:

	XY8Y-1										XY-11-2													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
5	N-ter	A	S	T	D	Y	H	Q	Y	H	T	D	G	G	G	I	V	N	A	V	N	G	S	G
	5'-	CT	AGT	ACA	GAT	TAT	TGG	CAA	TAT	TGG	ACA	GAC	GGT	GGC	GGT	ATC	GTT	AAT	GCC	GTG	AAC	GGC	T	
		A	TGT	CTA	ATA	ACC	GTT	ATA	ACC	TGT	CTG	CCA	CCG	CCA	TAG	CAA	TTA	CGG	CAC	TTG	CCG	AGG	CC	
		NheI									XY8Y-2					XY-16-1					BspEI			

(2) TS6a mutant, where threonine-3 (T-3), aspartic acid-4 (D-4) and asparagine-8 (N-8) have been converted to glycine (G), tyrosine (Y) and tyrosine (Y), respectively.

The oligonucleotides for cassette mutagenesis are XY3G4, 8Y-1; (SEQ ID NO:19) XY3G4, 8Y-2 (SEQ ID NO:20); XY-11-2 and XY-16-1 wherein the first two oligonucleotides are shown below:

	XY3G4, 8Y-1													
	1	2	3	4	5	6	7	8	9	10	11	12	13	
20	N-ter	A	S	G	Y	Y	H	Q	Y	H	T	D	G	G
	5'-	CT	AGT	GGA	TAC	TAT	TGG	CAA	TAT	TGG				
		A	CCT	ATG	ATA	ACC	GTT	ATA	ACC	TGT	CTG	CCA	CCG	
25		NheI			XY3G4, 8Y-2									

(3) TS3a mutant was prepared from a pair of oligonucleotides with mixed bases at codons-4 and 8. The oligonucleotides for cassette mutagenesis are XY(1-8)Mu-1 (SEQ ID NO:21), XY(1-8)Mu-2 (SEQ ID NO:22), XY-11-2 and XY-

16-1 wherein the first two oligonucleotides are shown below:

					XY(1-8)Mu-1									
5		1	2	3	4	5	6	7	8	9	10	11	12	13
	N-ter	A	S	T	D/Y	Y	W	Q		W	T	D	G	G
	5'-	CT	AGT	ACA	TAC	TAC	TGG	CAA	Tk1	TGG				
		_____A TGT CTG ATG ACC GTT Am1 ACC TGT CTG CCA CCG												
		NheI				XY(1-8)Mu-2								

k, l, m are mixed bases used in synthesis of oligonucleotide.

k = T+A+G

l = C+G

m = T+A+C

4) TS3 mutant was constructed by combining the mutations from TS1 with that from TS3a. The plasmid pXYbc was digested with Ssp I, Hind III and Avr II. Two fragments from this digest were isolated, a 2 KB Ssp I - Hind III (the vector portion of pXYbc) and a 245 bp Ssp I (a small portion of the vector and the first 78 codons of TS3a). A second plasmid pcW::TS1 was digested with Ssp I and Hind III and a 345 bp fragment was isolated (codons 79 - 185 of TS1). These three fragments were mixed together and ligated. After transformation, clones were picked from RBBX-agar plates if they produced clearing zones (xylanase activity). A clone was analyzed by DNA sequencing and was found to contain the desired mutations. This clone was designated TS3.

CHARACTERIZATION OF THE PROTEIN PRODUCTS

Protein purification

Protein samples were prepared from cells by first making an extract of the cells by grinding 10 g of the cell paste with 25 g of alumina powder. After grinding to a smooth mixture, small amounts (5 ml) of ice cold buffer A

(10mM sodium acetate, pH 5.5) were added and the mixture ground vigorously between additions. DNase, 10 μ g/ml, was added to lower the viscosity of the extract. The alumina and cell debris were removed by centrifugation of the mixture at 8000 x g for 30 min. The supernatant (25 ml) was then dialyzed overnight at 4°C against 3 L buffer A, using dialysis tubing with a 3500 molecular weight cutoff. A slight precipitate formed in the dialysis bag, which is removed by centrifugation at 8000 x g for 15 min.

The cell extract was then pumped onto a 50 ml bed volume, S-sepharose fast flow, cation exchange column (Kabi-Pharmacia, Canada), equilibrated in buffer A. The xylanase was eluted with a 300 ml linear gradient of 0 to 0.3 M NaCl in buffer A at a flow rate of 3 ml/min. The xylanase elutes at 100 to 150 ml of the gradient. The fraction are checked on SDS-PAGE, and those fractions having most of the xylanase were pooled, and concentrated by ultrafiltration using 3000 dalton molecular weight cutoff membranes (Amicon YM3). The concentrated material, 5 ml, was then applied to a 1.5 cm x 85 cm TSK-HW50S gel filtration column, equilibrated in 50 mM ammonium acetate pH 6. The xylanase eluted at a volume of 90 to 100 ml. These fractions were analyzed by SDS-PAGE, and the peaks pooled as pure xylanase. The protein was quantified using the extinction co-efficient at 280 nm. ϵ 0.1% solution = 4.08. Typical purified yield from 10 g of cells was 25 mg of xylanase.

Detection of free thiol groups

Two methods were used to indicate the presence of the SS bond. The first was shown in Figure 10. The electrophoretic mobility of the mutant proteins is faster under non-reducing conditions since the reduced protein is fully denatured and binds more SDS. This has also been observed for other disulfide bond containing proteins

(Mitchison and Wells, 1989, Biochemistry 28:4807-4815; Eder and Wilmanns, 1992, Biochemistry 31:4437-4444).

5 The second method checked for reactive sulfhydryl groups (SH groups). Approximately 200 μ g of protein (10 nmol) were used for each determination. The reaction was performed in cuvettes at room temperature. The reaction mixture contained 6M urea, 50 mM Tris-HCl, pH 8, 1 mM EDTA, and 9 - 13 nmol of xylanase, in a final volume of 1 ml.

10 The reaction was initiated by the addition of 10 μ l of 10 mM 5,5'-dithiobis(2-nitrobenzoic acid), Ellmans reagent. The A_{412} of the solution was monitored for 45 min. The amount of free thiol was calculated from the liberated 2-nitro-5-thiobenzoate anion, using a molar extinction

15 coefficient of 13,700. A single thiol containing mutant (S100C) was the positive control.

 Titration of these and other mutants with Ellman's reagent under denaturing conditions shows

20 undetectable levels of SH groups in the SS bond mutants, but shows stoichiometric amounts in a control containing a single SH group (Table 3). This shows that two of the mutants of the present invention (TS1 and TS2) have their

25 cysteine residues in SS bridges.

Table 3.
Determination of free sulfhydryl groups in xylanase
mutants

PROTEIN	[PROTEIN] μM (A_{280})	[SULFHYDRYL] μM	[SH]/ [PROTEIN]
BCX wild type	9.4	0	0
S100C	9.55	10.6	1.10
TS1	10.4	0	0
TS2	11.5	0	0
Mixture of S179C monomer and dimer	13.3	3	0.23

Measurement of enzymatic activity

The activity of the enzyme was measured two ways. The quantitative assay determined the number of reducing sugar ends generated from soluble xylan. The substrate for this assay was the fraction of birchwood xylan which dissolved in water from a 5% suspension of birchwood xylan (Sigma Chemical Co). After removing the insoluble fraction, the supernatant was freeze dried and stored in a desiccator. The measurement of specific activity was performed as follows. Reaction mixtures containing 100 μl of 30 mg/ml xylan in assay buffer (50 mM sodium citrate pH 5.5), 150 μl assay buffer, 50 μl of enzyme diluted in 1 mg/ml BSA, in assay buffer. The substrate and buffer were mixed and prewarmed at 40°C. The reaction was started by the addition of the enzyme. At various time intervals 50 μl portions were removed and the reaction stopped by diluting in 1 ml of 5 mM NaOH. The amount of reducing sugars was determined with the hydroxybenzoic acid hydrazide reagent (HBAH) (Lever, 1972, Analytical Biochem 47:273-279). A unit of enzyme activity was defined as that

amount generating 1 μ mol reducing sugar in 1 minute at 40°C. For the determination of kinetic parameters substrate concentrations from 0.4 mg/ml to 20 mg/ml were used. Kinetic parameters were calculated using the computer program Enzfitter (Leatherbarrow 1987, Enzfitter, a non-linear regression data analysis program for the IBM-PC. Elsevier Science Publishers BV. Amsterdam, The Netherlands. 1987).

The second assay for activity was used for relative measurement, i.e. residual activity after heat treatment. This assay was performed with RBBX (Remazol Brilliant Blue Xylan) as the substrate (Biely et al, 1987, Methods in Enzymology 160: 536-541). 100 μ l of 10 mg/ml RBBX in H₂O was mixed with 100 μ l of 100 mM ammonium acetate pH 6, and the mixture prewarmed to 40°C. The reaction was started by the addition of suitably diluted enzyme. After a fixed length of time, 5 or 10 min, the reaction was stopped by the addition of 0.5 ml 95% ethanol. The mixture was inverted to mix, and then allowed to stand at least 10 min. at room temperature. The mixture was then centrifuged in a microcentrifuge for 3 min. at 12,000 X g. The A₅₉₅ of the supernatant was measured.

Thermostability assay

To determine the thermostability of the mutant and wild type enzyme, the following parameters were used. The proteins were diluted to between 100 to 150 μ g/ml, in dilution buffer (50 mM ammonium acetate pH 6.0). 400 μ l of this solution were incubated in a 1.5 ml microcentrifuge tube, in a heating block containing glycerol. Portions of the solution were removed at specified times and immediately diluted 1 to 20 in dilution buffer and kept at room temperature until all samples had been taken. Portions of these diluted samples were then assayed for residual enzyme activity, using the RBBX assay. Results were expressed as percent residual activity compared to the



zero time point sample. Heating blocks were calibrated with a thermocouple and the measured temperature was that of the enzyme solution.

5 The data shown in Figures 11-16, clearly indicate
the thermostabilizing effect of the introduction of non-
native disulfide bridges into BCX. The mutant TS1 is
clearly stable at 61°C for up to 3 h. The second SS bond
mutant TS2 is not quite as stable, but maintains som
10 activity after 1 h at 61°C (see Figure 12). Figures 11 and
12 show curves for the mixed TS4 monomer/dimer preparation,
which is more stable than wild type but less stable than
TS1. It is however, more relevant to examine the
individual components. The mutant which contains only the
15 inter-molecular SS bond (TS4a) shows increased
thermostability at 58°C (Figure 13), and at this
temperature is as stable as the intra-molecular SS bond
mutant TS1 (Figure 14).

20 TS4 protein is produced as a mixture, but the
monomer (TS4M) and the dimer (TS4D) are easily separated by
rechromatographing the mixture on a cation exchange column.
TS4M behaves very much like the TS1 mutant, whereas TS4D
results in additive thermostability such that TS4D is more
25 stable than TS1. (Figures 14, 15 and 16).

30 There has been another example of an artificial
inter-molecular dimer using an SS bond, where the
thermostability was increased, however this protein was not
an enzyme, and the measurement of thermostability did not
include a biological activity assay (Sauer et al, 1986,
Biochemistry 25:5992-5998). The increase in
thermostability seen in the intra-molecular SS bond mutants
is similar to the effects seen in other proteins with an
35 engineered intra-molecular SS bond; however, there is no
significant decrease in specific activity, or change in
kinetic parameters (Table 4), as is sometimes the case with

SS bond mutants (Kanaya et al, 1991, Journal of Biological Chemistry 266(10):6038-6044).

Table 4
Kinetic Parameters of Thermostable Xylanase Mutants

MUTANT	K_m (mg/ml)	V_{max} (μ mol/min/ mg)	k_{cat}/K_m
Wild type BCX	1.78 ± 0.08	364 ± 24	11.04
Wild type BSX	1.86 ± 0.07	386 ± 14	10.16
TS1	1.72 ± 0.04	353 ± 5	10.07
Wild type BCX [*]	2.21 ± 0.27	456 ± 46	10.086
TS2 [*]	2.14 ± 0.24	413 ± 20	9.359
TS3 [*]	2.27 ± 0.22	269 ± 1.4	5.819

* These values were determined with a different batch of substrate, than the first 3 were, which accounts for the difference in K_m and V_{max}

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The decrease in the k_{cat}/K_m for TS3 indicates that some effect on catalysis and/or substrate specificity has occurred (Table 4). There is also a decrease in specific activity seen in TS4a and TS4D but this is not likely a severe limitation because decrease in the ability to hydrolyze soluble xylan may not be indicative of how well the protein performs in pre-bleaching applications on pulp (Table 5). The activity of the thermostable mutants is higher at elevated temperatures (Figure 17).

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Table 5
Specific Activity of the Most Stable Mutants of the
B. circulans Xylanase

MUTATION	SPECIFIC ACTIVITY ^a (% OF WILD TYPE)
TS1	105
TS2	86
TS3a	77
TS3	61
TS4a	59
TS4M	97
TS4D	66
TS5a	93
TS6a	103

^aThese activities were determined using the reducing sugar assay (HBAH), and are the average of at least two determinations.

5

The N-terminal mutations, were found to confer thermostability, although less than that seen with the SS bond mutants. Thermostability of these mutants was determined in two ways: by a residual activity assay and by scanning calorimetry.

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In the residual activity assay identical samples of a xylanase mutant were preheated in the assay buffer (50mM sodium citrate, pH 6.2) in Eppendorf tubes at different temperatures. The Eppendorf tubes with samples were heated in small water baths with lids. The heating temperatures were determined by a digital thermometer with a thermocouple sensor which measured to 0.1°C. After 30 min., samples were cooled down to 20°C before being assayed at 40°C. The residual enzyme activity of the heated sample

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was expressed as a percentage of the activity of an unheated sample. This residual activity was plotted against the heating temperature (Figure 18). From the plot, the $T_{1/2}$ the preheating temperature, at which the xylanase still retained 50% of its activity, was determined and is shown in Table 6.

TABLE 6

$T_{1/2}$ of pre-heating temperatures at which xylanase will retain 50% of activity

Xylanase	$T_{1/2}$ (°C)
BCX (wild type)	53.5
TS3a	56.5
TS5a	55.5
TS6a	58.5

Samples of the xylanase were studied by scanning calorimetry to study the unfolding process of the xylanase structure as it relates to the rising temperature. Then T_m , the temperature at which half of the xylanase molecules have been denatured or melted, was determined. A higher T_m reflects a more thermostable molecule. It should be emphasized that calorimetry is concerned with the maintenance of the molecular structure, not enzymatic activity. However, the loss of enzyme activity through heating is often associated with the collapse of the molecular structure. The melting temperatures, T_m of wild type and mutant xylanases were determined from the calorimetric scans and are shown in Table 7.

TABLE 7
Melting temperature T_m of xylanases

Xylanase	T_m ($^{\circ}\text{C}$)
BCX (wild type)	59.7
TS3a	62.7
TS5a	62.0
TS6a	64.6

Residue-8 appears to be essential to the thermostability of the BCX. The mechanism of the effect of this mutation may be explained by the 3-dimensional structure which reveals that a space existed between asparagine-8 and the other residues (Figure 19). This space was occupied by two water molecules in the wild-type enzyme (BCX). Molecular modelling indicated that substitution of asparagine-8 by phenylalanine or tyrosine could displace the water molecules (Figure 20). Increased thermostability resulting from this substitution may be a result of increased hydrophobic interaction contributed by these larger hydrophobic side-chains. The aromatic ring may displace the buried water molecules thus gaining hydrophobic interaction. In addition, the phenolic hydroxy group may also form a hydrogen bond with the carbonyl of peptide linkage-16 on the main chain.

The mutations at the N-terminus, described above, in combination with one of the SS bond mutations, resulted in an additive thermostability (Figure 14, 15 and 16). The combination of mutations in TS3 result in a protein with a thermostability of 64°C .

X-ray Crystallographic Structure of the xylanases from
Bacillus circulans and *Trichoderma harzianum*

Structure of the *B. circulans* xylanase

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Crystals of the *B. circulans* xylanase were grown by the hanging drop vapour diffusion method. The reservoir buffer was 40mM Tris, pH 7.5, 22% saturated $(\text{NH}_4)_2\text{SO}_4$ and 100mM NaCl. Droplets were seeded after one day of equilibration. The space group of the crystals was $P2_12_12_1$. The unit cell parameters for all structures are given in Table 8. The heavy-atom derivative was obtained by soaking crystals of the Ser100Cys mutant protein in 10mM HgCl_2 for 6 days. All of the X-ray diffraction data sets for both the *B. circulans* and *T. harzianum* xylanase crystals were collected on a San Diego Multiwire Area Detector system on a Rigaku rotating anode generator.

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All data reduction was performed using the San Diego software and the PHASES program package (Furey, W. & Swaminathan, S. (1990) "PHASES - A Program Package for the Processing and Analysis of Diffraction Data from Macromolecules", PA33, American Crystallographic Association Meeting Abstracts, Series 2, 18, pg 73). The initial electron density map for the *B. circulans* xylanase was calculated from phases based on the native (wild-type) data set and the positions of the mercury atoms found from the Patterson maps for the data collected on the HgCl_2 derivative of the Ser100Cys mutant protein. The initial electron density map was "skeletonized" using BONES (Greer, J. (1985) Methods in Enzymology 115, 206) and the initial model was built with TOM/FRODO (Jones, T. (1978) J. Appl. Cryst. 11, 268) and with O (Jones, T.A., Bergdoll, M., & Kjeldgaard, M. (1990) O: A macromolecular modelling environment. In "Crystallographic and Modelling Methods in Molecular Design" (Bugg, C.E. & Ealick, S.E., Editors).

Springer-Verlag, New York). All refinements were carried out using the simulated annealing and minimization protocols of X-PLOR (Brunger, A.T. (1988) J. Mol. Biol. 203, 803).

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Structure of TS1 mutant of the *B. circulans* xylanase

Crystals of the TS1 mutant were grown as for the wild-type enzyme and were isomorphous with the crystals of the wild-type enzyme. A model for the cysteine side-chains was built into a difference electron density map that was calculated with data measured from the TS1 crystals and with phases calculated from the refined model of the wild-type structure.

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Structure of the *T. harzianum* xylanase

Crystals of the *T. harzianum* xylanase were grown by the hanging drop vapour diffusion method. The reservoir buffer was 16mM Tris, pH 7.5, 20% saturated $(\text{NH}_4)_2\text{SO}_4$. Droplets were seeded after one day of equilibration. The space group of the crystals was also $P2_12_12_1$ but with different unit cell dimensions and with a different crystal packing arrangement than for the *B. circulans* crystals.

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The structure was solved by standard molecular replacement methods with the programs MERLOT (Fitzgerald, P.M.D. (1988) J. Appl. Cryst. 21, 273-278) and BRUTE (Fujinaga, M. and Read, R. (1987) J. Appl. Crystallogr., 20, 517-521) using the *B. circulans* xylanase as the search model. Refinement statistics for all structures are given in Table 9 and plots of average main-chain B-factors for the three structures are shown in Figures 21, 22 and 23. Ramachandran diagrams indicating the stereochemical quality of the structures are shown in Figures 24 and 25.

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Table 8
Data collection statistics

Data Set	<i>B. circulans</i>			<i>T. harzianum</i>
	Wild-type	S100C mutant + HgCl ₂	TS1	Wild-type
Unit cell parameters (Å)				
a	44.00	43.96	43.90	43.67
b	52.78	52.71	52.88	94.65
c	78.39	78.41	78.43	51.55
Resolution (Å)	1.6	2.3	1.6	1.8
Merging R-factor (R_{sym})	0.028	0.062	0.062	0.111
Completeness of data set to resolution limit	94%	99%	99%	98%
Isomorphous difference (R_{iso})	n/a	0.098	0.077	n/a
Figure of merit	n/a	0.77	n/a	n/a

where,

$$R_{sym} = \frac{\sum |\langle I \rangle - I_{obs}|}{\sum I_{obs}}$$

$\langle I \rangle$ is the average intensity for a particular reflection and I_{obs} is one intensity measurement for that reflection.

$$R_{iso} = \frac{\sum |F_{deriv} - F_{nat}|}{\sum |F_{nat}|}$$

F_{deriv} and F_{nat} are the amplitudes of the structure factors for the derivative (S100C + HgCl₂ and TS1) and native (wild-type) data sets, respectively.

5

n/a = not applicable to this data set

Figure of merit is a measure of the quality of a derivative for calculating phases.

Table 9
Refinement statistics

Data Set	<i>B. circulans</i>		<i>T. harzianum</i>
	Wild-type	TS1	Wild-type
Number of non-hydrogen protein atoms	1448	1446	1473
Solvent molecules	141 waters + 1 sulfate	152 waters	59 waters
R-factor	0.163	0.172	0.208
RMS-deviations from ideality for			
bonds (Å):	0.009	0.009	0.010
angles (°):	1.691	1.783	1.318
dihedrals (°):	27.371	27.525	30.016
impropers (°):	1.312	1.351	2.326

where,

$$R\text{-factor} = \frac{\sum |F_{calc} - F_{obs}|}{\sum |F_{obs}|}$$

F_{calc} and F_{obs} are the amplitudes of the structure factors that are calculated from the refined model structure and from the measured reflections, respectively.

5

EXAMPLE 5CONSTRUCTION OF OTHER MUTATIONS AT THE N-TERMINUS OF B. CIRCULANS XYLANASE

5 Additional N-terminal mutants have been
constructed and tabulated (Table 10). Construction of
mutants TS7a, TS8a, TS9a, TS10a, TS11a, TS12a, TS13a,
10 TS14a, TS15a, TS16a, TS17 and TS19a has been accomplished
via the identical protocol of cassette mutagenesis which
previously yielded TS3a, TS5a and TS6a as described in
Example 4 of the application. This involved ligation of
various oligonucleotides to the NheI/BspEI linearized
15 plasmid pXYbc (Figure 9). Another mutant TS18a was also
prepared via the same protocol with the NheI/BamHI
linearized plasmid pXYbc. Different overlapping
oligonucleotides encoding various mutation have been
synthesized.

20 (a) TS7a mutant, where asparagine-8 has been converted to
phenylalanine. The oligonucleotides for cassette
mutagenesis are XY8F-1 (SEQ ID NO:23), XY8F-2 (SEQ ID
NO:24), XY-11-2 (SEQ ID NO:17) and XY-16-1 (SEQ ID NO:18).

XY8F-1 (SEQ ID NO:23)

25 1 2 3 4 5 6 7 8 9
A S T D Y H Q F H

5'-CT AGT ACA GAT TAT TGG CAA TTC TGG

A TGT CTA ATA ACC GTT AAG ACC TGT CTG CCA CCG

XY8F-2 (SEQ ID NO:24)

30

(b) TS8a mutant, where asparagine-8 has been converted to
tryptophan. The oligonucleotides for cassette mutagenesis
are XY8W-1 (SEQ ID NO:25), XY8W-2 (SEQ ID NO:26), XY-11-2
(SEQ ID NO:17) and XY-16-1 (SEQ ID NO:18).

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XY8W-1 (SEQ ID NO:25)

1	2	3	4	5	6	7	8	9
A	S	T	D	Y	W	Q	W	W

5'-CT AGT ACA GAT TAT TGG CAA TGG TGG

A TGT CTA ATA ACC GTT ACC ACC TGT CTG CCA CCG

XY8W-2 (SEQ ID NO:26)

(c) TS9a mutant, where aspartic acid-4 has been converted to tyrosine. The oligonucleotides for cassette mutagenesis are XY4Y-1 (SEQ ID NO:27), XY4Y-2 (SEQ ID NO:28), XY-11-2 (SEQ ID NO:17) and XY-16-1 (SEQ ID NO:18).

XY4Y-1 (SEQ ID NO:27)

1	2	3	4	5	6	7	8	9
A	S	T	Y	Y	W	Q	N	W

5'-CT AGT ACA TAC TAC TGG CAG AAC TGG

A TGT ATG ATG ACC GTC AAG ACC TGT CTG CCA CCG

XY4Y-2 (SEQ ID NO:28)

(d) TS10a mutant, where aspartic acid-4 and asparagine-8 have both been converted to tyrosine. The oligonucleotides for cassette mutagenesis are XY4,8Y-1 (SEQ ID NO:29), XY4,8Y-2 (SEQ ID NO:30), XY-11-2 (SEQ ID NO:17) and XY-16-1 (SEQ ID NO:18).

XY4,8Y-1 (SEQ ID NO:29)

1	2	3	4	5	6	7	8	9
A	S	T	Y	Y	W	Q	Y	W

5'-CT AGC ACA TAC TAT TGG CAA TAT TGG

G TGT ATG ATA ACC GTT ATA ACC TGT CTG CCA CCG

XY4,8Y-2 (SEQ ID NO:30)

(e) TS11a mutant, where aspartic acid-4 and asparagine-8 have been converted to tyrosine and tryptophan respectively. The oligonucleotides for cassette mutagenesis are XY4Y8W-1 (SEQ ID NO:31), XY4Y8W-2 (SEQ ID NO:32), XY-11-2 (SEQ ID NO:17) and XY-16-1 (SEQ ID NO:18).



XY4Y8W-1 (SEQ ID NO:31)

1	2	3	4	5	6	7	8	9
A	S	T	Y	Y	W	Q	W	W

5'-CT AGC ACA TAC TAT TGG CAA TGG TGG

5

G TGT ATG ATA ACC GTT ACC ACC TGT CTG CCA CCG

XY4Y8W-2 (SEQ ID NO:32)

(f) TS12a mutant, where threonine-3 has been converted to glycine. The oligonucleotides for cassette mutagenesis are XY3G-1 (SEQ ID NO:33), XY3G-2 (SEQ ID NO:34), XY-11-2 (SEQ ID NO:17) and XY-16-1 (SEQ ID NO:18).

10

XY3G-1 (SEQ ID NO:33)

1	2	3	4	5	6	7	8	9
A	S	G	D	Y	W	Q	N	W

15

5'-CT AGC GGA GAC TAT TGG CAG AAT TGG

G CCT CTG ATA ACC GTT TTA ACC TGT CTG CCA CCG

XY3G-2 (SEQ ID NO:34)

(g) TS13a mutant, where threonine-3 and aspartic acid-4 have been converted to glycine and tyrosine respectively. The oligonucleotides for cassette mutagenesis are XY3G4Y-1 (SEQ ID NO:35), XY3G4Y-2 (SEQ ID NO:36), XY-11-2 (SEQ ID NO:17) and XY-16-1 (SEQ ID NO:18).

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XY3G4Y-1 (SEQ ID NO:35)

1	2	3	4	5	6	7	8	9
A	S	G	Y	Y	W	Q	N	W

5'-CT AGC GGA TAC TAT TGG CAG AAT TGG

30

G CCT ATG ATA ACC GTT TTA ACC TGT CTG CCA CCG

XY3G4Y-2 (SEQ ID NO:36)

(h) TS14a mutant, where threonine-3, aspartic acid-4 and asparagine-8 have been converted to glycine, tyrosine and phenylalanine respectively. The oligonucleotides for cassette mutagenesis are XY3G4Y8F-2 (SEQ ID NO:37), XY3G4Y8F-3 (SEQ ID NO:38), XY-11-2 (SEQ ID NO:17) and XY-16-1 (SEQ ID NO:18).

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XY3G4Y8F-2 (SEQ ID NO:37)

1 2 3 4 5 6 7 8 9
A S G Y Y W Q F W

5'-CT AGC GGA TAC TAT TGG CAA TTC TGG

5

G CCT ATG ATA ACC GTT AAG ACC TGT CTG CCA CCG

XY3G4Y8F-3 (SEQ ID NO:38)

(i) TS15a mutant, where serine-22 has been converted to proline. The oligonucleotides for cassette mutagenesis are XY-11-3 (SEQ ID NO:39), XY-16-3 (SEQ ID NO:40), XY22P-1 (SEQ ID NO:41) and XY22P-2 (SEQ ID NO:42).

XY-11-3 (SEQ ID NO:39)

1 2 3 4 5 6 7 8 9
A S T D Y W Q N W

15

5'-CT AGC ACC GAT TAC TGG CAG AAC TGG

G TGG CTA ATG ACC GTC TTG ACC TGT CTG CCA CCG

XY-16-3 (SEQ ID NO:40)

XY22P-1 (SEQ ID NO:41)

10 11 12 13 14 15 16 17 18 19 20 21 22 23
T D G G G I V N A V N G P G

20

5'-ACA GAC GGT GGC GGT ATC GTT AAT GCC GTG AAC GGC C

CCA TAG CAA TTA CGG CAC TTG CCG GGG CC

25

XY22P-2 (SEQ ID NO:42)

(j) TS16a mutant, where asparagine-8 and glycine-21 have been converted to phenylalanine and proline respectively. The oligonucleotides for cassette mutagenesis are XY8F-1 (SEQ ID NO:23), XY8F-2 (SEQ ID NO:24), XY21P-1 (SEQ ID NO:43) and XY21P-2 (SEQ ID NO:44).

XY21P-1 (SEQ ID NO:43)

10 11 12 13 14 15 16 17 18 19 20 21 22 23
T D G G G I V N A V N P S G

35

5'-ACA GAC GGT GGC GGT ATC GTT AAT GCC GTG AAC CCA T

CCA TAG CAA TTA CGG CAC TTG GGT AGG CC

XY21P-2 (SEQ ID NO:44)

(k) TS17a mutant, where asparagine-8 and serine-22 have been converted to phenylalanine and proline respectively. The oligonucleotides for cassette mutagenesis are XY8F-1 (SEQ ID NO:23), XY8F-2 (SEQ ID NO:24), XY22P-1 (SEQ ID NO:41) and XY22P-2 (SEQ ID NO:42).

40

(1) TS19a mutant, where threonine-3, aspartic acid-4, asparagine-8 and serine-22 have been converted to glycine, tyrosine, tyrosine and proline respectively. The oligonucleotides for cassette mutagenesis are XY3G4,8Y-1 (SEQ ID NO:19), XY3G4,8Y-2 (SEQ ID NO:20), XY22P-1 (SEQ ID NO:41) and XY22P-2 (SEQ ID NO:42).

(m) TS18a is a mutant where asparagine-8 and glycine-23 have been converted to phenylalanine and proline. The oligonucleotides for cassette mutagenesis in the NheI/BamHI linearized plasmid pXYbc are XY8F-1 (SEQ ID NO:23), XY8F-2 (SEQ ID NO:24), XY24P-1 (SEQ ID NO:45), XY23P-2 (SEQ ID NO:46), XY-12a (SEQ ID NO:47) and XY-15a (SEQ ID NO:48). The plasmid obtained was subcloned to yield TS18a.

XY24P-1 (SEQ ID NO:45)

```

10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
  T  D  G  G  G  I  V  N  A  V  N  G  S  G  P
5'-ACA GAC GGT GGC GGT ATC GTT AAT GCC GTG AAC GGC TCC GGA CCA
  CCA TAG CAA TTA CGG CAC TTG CCG AGG GGC CCT
  XY23P-2 (SEQ ID NO:46)                P  G

```

```

25 26 27 28 29 30 31 32 33 34 35 36 37 38 39
  N  Y  S  V  H  H  S  H  T  G  H  F  V  V  G
-AAT TAT AGC GTC AAT TGG TCT AAT ACT GGG AAC TTC GTA GTC GGA
-TTA ATA TCG CAG TTA ACC AGA TTA TGA CCC TTG AAG CAT CAG CCT

```

XY-12a (SEQ ID NO:47)

```

40 41 42 43 44 45
  K  G  H  T  T  G
-AAA GGT TGG ACG ACA G
-TTT CCA ACC TGC TGT CCT AG

```

XY-15a (SEQ ID NO:48)

(n) TS20a mutant with extension from both the N-terminus (glycine-(-1)) and from the C-terminus (glycine-186 and cysteine-187), has conversion of alanine-1 into cysteine. Its construction was accomplished via a 2-step protocol identical to that described in Example 1 of the application. Initially this involved a polymerase chain reaction (PCR) with the template plasmid pXYbc (Figure 9)

and primers XY(-1)G1C (SEQ ID NO:49) and XY186G187C (SEQ ID NO:50). Subsequently the Nde/HindIII linearized PCR product was ligated into the identically linearized plasmid pCWBCX3' SYN.

5

XY(-1)G1C (SEQ ID NO:49)

NdeI -1 1 2 3 4 5 6
st G C S T D Y W

5'-CAT CGA TGC TTA GGA GGT CAT ATG GGA TGT AGC ACA GAT TAC TGG

10

7 8

Q N

-CAA AAC-3'

XY186G187C (SEQ ID NO:50)

15

179 180 181 182 183 184 185 186 187

S S N V T V W G C ter HindIII3'-GA AGG TTG CAA TGT CAC ACC CCA ACG ATT TCT AGA ACT TCG AAT AGC

-TAC TAT TCG ACA-5'

20

(o) TS21a mutant which has extension from both the N-terminus (glycine-(-1)) and from the C-terminus (glycine-186 and cysteine-187), has conversion of alanine-1 and asparagine-8 into cysteine and phenylalanine respectively. Its construction was accomplished with the protocol described for TS20a, with differences in the PCR template (plasmid of TS7a; primers XY(-1)G1C8F (SEQ ID NO:51) and XY186G187C (SEQ ID NO:50)).

30

XY(-1)G1C8F (SEQ ID NO:51)

NdeI -1 1 2 3 4 5 6
st G C S T D Y W

5'-CAT CGA TGC TTA GGA GGT CAT ATG GGA TGT AGT ACA GAT TAT TGG

35

7 8

Q F

-CAA TTC-3'

Tablo 10
Xylanase N-terminal mutants

Name	Mutations	Type of Mutation
TS3a	D4Y N8F	N-terminal mutation
TS5a	N8Y	N-terminal mutation
TS6a	T3G D4Y N8Y	N-terminal mutation
TS7a	N8F	N-terminal mutation
TS8a	N8W	N-terminal mutation
TS9a	D4Y	N-terminal mutation
TS10a	D4Y N8Y	N-terminal mutation
TS11a	D4Y N8W	N-terminal mutation
TS12a	T3G	N-terminal mutation
TS13a	T3G D4Y	N-terminal mutation
TS14a	T3G D4Y N8F	N-terminal mutation
TS15a	S22P	N-terminal mutation
TS16a	N8F G21P	N-terminal mutation
TS17a	N8F S22P	N-terminal mutation
TS18a	N8F G23P	N-terminal mutation
TS19a	T3G D4Y N8Y S22P	N-terminal mutation
TS20a	(-1)G A1C 186G 187C	N/C-terminal SS bond
TS21a	N8F (-1)G A1C 186G 187C	N-terminal mutation N/C-terminal SS bond

Expression, extraction and purification

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The expression, extraction, purification and assay processes for the mutant xylanases were identical to the protocols described in Example 4 of the application. The mutant xylanases have shown specific enzyme activity 10 close (70% - 100%) to the wild type BCX.

Thermostability assay

Thermostability assay was identical to that described for the N-terminal mutant enzymes previously described in Example 4 of application, with a major difference in equipment used in the assay. The water bath for incubating enzymes in Example 4 has a fluctuation of $\pm 1.5^{\circ}\text{C}$, while the circulating water bath (Haake type F 4391) used in the present examples fluctuated at $\pm 0.1^{\circ}\text{C}$. The new water bath should therefore yield more accurate data in subsequent assay. Enzyme was initially incubated in buffer (50mM sodium citrate, pH 5.5) without substrate (xylan) at a set temperature for 30 min. The residual enzymic activity was then determined at a lower temperature of 40°C via hydrolysis of soluble birchwood xylan, with the reducing sugar estimated by the hydroxybenzoic hydrazide reagent (HBAH). The thermostability of BCX and the earlier mutants TS1, TS2, TS3, TS3a, TS5a and TS6a has been reevaluated using the new equipment (Table 11).

The thermostability temperature $T_{1/2}$ at which various xylanase mutants retain 50% of activity was determined. The differences between the $T_{1/2}$ of mutants and wild type BCX have been tabulated (Table 11). The discrepancies in the $T_{1/2}$ values of the earlier mutants in Table 6 (of the parent application) and Table 11 were most likely due to the differences in performance of the two water baths. The newly established $T_{1/2}$ of BCX is 55°C , as compared to an earlier value of 53.5°C in Table 6.

Various mutations N8F (in TS7a, TS3a, TS14a), N8Y (in TS5a, TS6a, TS10a) and S22P (in TS15a, TS17a, TS19a), alone or in combination, caused a moderate increase in $T_{1/2}$ of $2-4^{\circ}\text{C}$, as compared to the greater gain of $5-8^{\circ}\text{C}$ by the internal or N/C-terminal disulfide bond (in TS1, TS2, TS3, TS20a).

Temperature optimal and pH optimum in soluble xylan

5 The temperature optimum assay was carried out substantially as for thermostability determinations except instead of incubating the enzymes in buffer without xylan for 30 min., xylanase is incubated in the same manner with xylan in the buffer. The modified process is designed to evaluate the hydrolysis of soluble xylan by the mutant enzyme at different temperatures for 30 min. The reducing sugar released was then determined by the HBAH reagent.

10 Higher temperature exerted dramatically different effects on the hydrolysis of soluble xylan by wild type BCX and mutants (Figure 26). The temperature optimum T_{opt} is defined as the highest temperature at which 150% relative enzymic activity was maintained as compared to performance at 40°. The temperature optimum T_{opt} of BCX is 60°C. The change of temperature optimum of mutants versus wild type BCX was tabulated (Table 11).

20 Mutations such as N8Y (in TS5a, TS10a), N8F (in TS7a, TS3a), S22P (TS15a, TS17a), with only minor gain of 2-3°C in the thermostability assay, caused an elevation of T_{opt} by 5°C (Table 11). The positive effect of mutations N8Y and N8F indicates that the aromatic residues tyrosine and phenylalanine are advantageous to the T_{opt} . However, the mutation to another aromatic residue tryptophan (N8W in mutants TS8a and TS11a) lowered the T_{opt} by 4-5°C. While the mutation S22P together with N8F elevated the T_{opt} by 10°C in mutant TS17a, a similar conversion of the neighbouring residues to proline (G21P and G23P) dramatically lowered the T_{opt} of TS16a and TS18a by as much as 11°C.

35 In contrast, the internal disulfide (in TS1, TS2), with a gain of 5-8°C in thermostability assay, demonstrated no gain in T_{opt} (Table 11). The N/C-terminal

disulfide bond (in TS20a) with good thermostability of 5°C has only a moderate elevation of 3°C in T_{op} (Table 11).

5 The mutations T3G (in TS12a) or D4Y (in TS9a)
independently caused a decrease of 3-9°C in T_{op} (Table 11).
However, the combination of this pair of seemingly damaging
mutations T3G and D4Y, with N8Y generated mutant TS6a which
demonstrated a T_{op} increase of 4°C as compared to TS5a
(N8Y). On the other hand, this conversion of mutant TS5a
10 to TS6a resulted in a net loss of thermostability (1°C).
Such opposite effect on thermostability and temperature
optimal was also repeated in the conversion of mutant TS7a
to TS14a. With a further addition of mutation S22P in
mutant TS19a, an elevation of T_{op} as much as 14°C has been
15 achieved. However, despite this gain in the T_{op} , the total
gain of thermostability ($T_{1/2}$) remained not more than 4°C.

 There is no clear correlation between the
thermostable temperature ($T_{1/2}$) determined from incubation
20 without substrate and the temperature optimum (T_{op}) in the
assay with soluble xylan (Table 11). Therefore, a gain in
thermostability does not necessarily correlate with a gain
in temperature optimum to hydrolyse xylan or to bleach
pulp.

25 The functional pH (pH optimum) of mutant enzymes
was determined. Initially the enzyme was incubated in
buffers of various pH without substrate at 50°C for 20 hr.
Then the enzymic activity of the incubated enzyme was
30 determined via the 4 min. 40°C assay conducted in the
incubation buffer, instead of the 50mM sodium citrate (pH
5.5) normally used for such assay (Example 4). The pH
optimum (pH_{op}) is defined as the highest pH at which the
enzyme still maintains 50% of the maximal activity. Five
35 mutants TS5a, TS7a, TS17a, TS19a and TS20a with elevated T_{op}
were selected for this study. The enzymic activity of
these mutants was compared to wild type BCX at different pH

(Figure 27). BCX can only maintain maximal activity up to pH 5.5 while the selected mutants can endure up to pH 7. Therefore the pH optimum of these mutants have been increased by more than 1 pH unit (Table 11).

Table 11
Changes of thermostability, temperature optimum and pH
optimum of mutant xylanases in soluble xylan assay.

Name	Mutations	Type of Mutation	Buffer	Sol. xylan	
			$\Delta T_{1/2}$ °C	ΔT_{op} °C	ΔpH_{op}
BCX	wild type		0	0	0
TS1	S100C N148C	internal SS bond	8	0	
TS2	V98C A152C	internal SS bond	5	0	
TS3	S100C N148C D4Y N8F	internal SS bond N-term. mutation	11	5	
TS3a	D4Y N8F	N-term. mutation	2	5	
TS5a	N8Y	N-term. mutation	3	5	1.2
TS6a	T3G D4Y N8Y	N-term. mutation	2	9	
TS7a	N8F	N-term. mutation	3	5	1.2
TS8a	N8W	N-term. mutation	-2	-5	
TS9a	D4Y	N-term. mutation		-3	
TS10a	D4Y N8Y	N-term. mutation	2	5	
TS11a	D4Y N8W	N-term. mutation	-3	-4	
TS12a	T3G	N-term. mutation		-9	
TS13a	T3G D4Y	N-term. mutation		0	
TS14a	T3G D4Y N8F	N-term. mutation	2	9	
TS15a	S22P	N-term. mutation		5	
TS16a	N8F G21P	N-term. mutation		-11	
TS17a	N8F S22P	N-term. mutation	4	10	1.1
TS18a	N8F G23P	N-term. mutation		-10	
TS19a	T3G D4Y N8Y S22P	N-term. mutation	4	14	1.1
TS20a	(-1)G A1C 186G 187C	N/C-term. SS bond	5	3	1.1
TS21a	N8F (-1)G A1C 186G 187C	N-term. mutation N/C-term. SS bond		8	

In summary, the appropriate mutations (S22P, N/C-terminal disulfide bond, N8F and N8Y alone or in combination with T3G and D4Y) can permit the mutant xylanase to hydrolyse xylan at higher temperature and pH.

Bleaching of Pulp by Mutant Xylanases

Although the 30 min. soluble xylan assay determines the effectiveness of mutant xylanase in direct hydrolysis of xylan at high temperature, the usefulness of the enzyme as a bleaching agent can only be established via the pulp bleaching test. The protocol for such small scale test has been published in detail (Tolan and Canovas, 1992; Nissen et al, 1992, both incorporated herein by reference) and well-known to researcher in the field. Pulp suspension at different temperature or pH was treated with the enzyme for 2 hr. The bleaching effect was measured in brightness gain or whiteness of the pulp after bleaching. In this process, the temperature optimum (T_{ϕ}) is defined as the highest temperature at which the enzyme still achieves a brightness gain of 0.4 in the bleached pulp. The pH optimum (pH_{ϕ}) is defined as the highest pH at which the enzyme still achieved a brightness gain of 0.4 in the bleached pulp.

Several mutants were chosen for the pulp test at pH 8. While the wild type BCX functioned well at pH 7 with a temperature optimum of 54°C, it failed at pH 8 (Figure 28). In the same test at pH 8 (Table 12), mutants TS20a, TS17a and TS19a showed increase of T_{ϕ} by 3, 10 and 14°C, respectively over BCX (at pH 7). Thus the mutant xylanase TS19a can efficiently bleach pulp at temperatures as high as 68°C (T_{ϕ}). In addition to elevated temperature, the performance of these mutants at pH 8 also indicated an pH

upshift of 1 unit over BCX. Such gains in T_{op} and pH_{op} in pulp bleaching (Table 12) are in general agreement to the gains already determined through the soluble xylan assay (Table 11).

5

The mutant TS1, which has achieved greater thermostability ($T_{1/2}$) than the three mutants above (Table 11), was also tested for its effectiveness in pulp bleaching. However, its performance (temperature optimum of 54°C) was only equal to the wild type BCX (Table 12). This has already been predicted in the 30 min assay on soluble xylan (Table 11). The general lack of agreement between the thermostability ($T_{1/2}$) and the temperature optimal T_{op} in pulp bleaching (Table 12) or soluble xylan assay (Table 11) confirmed that greater thermostability may not be reflected in a better performance in pulp bleaching at elevated temperature.

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In conclusion, appropriate mutations (N8Y, N8F, S22P and N/C- terminal disulfide bond; the combination of T3G, D4Y and N8Y or N8F) at the N-terminus region (1-25) region are beneficial in the performance of the enzyme in pulp bleaching or other applications at higher temperature and pH.

20

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Table 12
Changes in Thermostability, Temperature Optimum and pH
Optimum of mutant xylanases in soluble xylan and pulp
bleaching.

Name	Mutations	Buffer	Soluble xylan		Pulp bleaching	
		$\Delta T_{1/2}$ °C	ΔT_{op} °C	ΔpH_{op}	ΔT_{op} °C	ΔpH_{op}
BCX	wild type	0	0	0	0	0
TS1	S100C N148C	8	0		0	
TS17a	N8F S22P	4	10	1.1	10	1
TS19a	T3G D4Y N8Y S22P	4	14	1.1	14	1
TS209a	(-1)G A1C 186G 187C	5	3	1.1	3	1

The invention has been described with reference to particular embodiments, although it is understood that the specific details shown are merely illustrative, and the invention may be carried out in other ways without departing from the spirit and the scope of the following claims.

THE EMBODIMENTS OF THE INVENTION IN WHICH AN EXCLUSIVE
PROPERTY OR PRIVILEGE IS CLAIMED ARE DEFINED AS FOLLOWS:

1. A modified family G xylanase essentially having the
5 structure of the *B. circulans* enzyme or mutated to
essentially have this structure, wherein said xylanase has
increased stability and wherein said xylanase is modified
through either the introduction of at least one non-native
10 disulfide bridge, the introduction of at least one N-
terminal mutation, or combinations thereof;

wherein the disulfide bridge is an intra-molecular
bridge between a cysteine amino acid, which has been
introduced on the last strand of beta-sheet III, and a
15 cysteine amino acid, which has been introduced on the alpha
helix, or on either side, adjacent to the alpha helix or
the disulphide bridge is an inter-molecular bridge between
two xylanase molecules, wherein a cysteine amino acid has
been introduced in each of said two molecules, on the
external region; and

20 wherein the N-terminal mutation is selected from at
least one mutation of the group consisting of the
introduction of tyrosine at amino acid position 8,
introduction of phenylalanine at amino acid position 8,
introduction of proline at amino acid position 22, and
25 introduction of an N-terminal to C-terminal disulfide
bridge, and wherein these N-terminal mutations can be used
in combination with other N-terminal mutation introduced at
amino acid position 1 to 25 of the N-terminal region, based
on the amino acid numbering from *B. circulans* xylanase.

30 2. A modified family G xylanase of Claim 1, wherein
said xylanase has increased stability as demonstrated by at
least one of an increase in thermostability, an increase in
temperature optimum, an increase in pH optimum, or
combinations thereof, as determined in the hydrolysis of
xylan or in the bleaching of pulp.

3. The modified xylanase of Claim 1, wherein the family G xylanase is selected from a bacterial or fungal xylanase.

5 4. The modified xylanase of Claim 3, wherein the bacterial xylanase is from bacteria selected from the group consisting of *Bacillus pumilus*; *Clostridium acetobutylicum*; *Ruminococcus flavefaciens*; *Streptomyces* sp.; *Streptomyces lividans*, B; *Streptomyces lividans*, C; *Bacillus circulans*; and *Bacillus subtilis*.

10 5. The modified xylanase of Claim 3, wherein the fungal xylanase is from fungi selected from the group consisting of *Trichoderma reesei*, II; *Trichoderma viride*; *Trichoderma harzianum*; *Schizophyllum commune*; *Aspergillus niger* var. *awamori*; *Aspergillus tubigenensis*, A; and *Trichoderma reesei*, I.

15 6. The modified xylanase of Claim 1, wherein the cysteine on the last strand of beta-sheet III is between amino acid residues 95 and 109 and the cysteine on the alpha-helix is between the amino acid residues from 143 to 158, based on the amino acid numbering from *B. circulans* xylanase.

20 7. The modified xylanase of Claim 1, wherein the disulfide bridge is an intra-molecular bridge between amino acids selected from the group consisting of 100 and 148, and 98 and 152, based on the amino acid numbering from *B. circulans* xylanase.

25 8. The modified xylanase of Claim 1, wherein the cysteine amino acid is introduced on an external region of the xylanase molecule selected from the regions consisting of beta-sheet I, the loop preceding the last strand of sheet III and beta-sheet III, and alpha-helix and surrounding loops.

30

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9. The modified xylanase of Claim 8, wherein the cysteine amino acid is introduced at a residue position selected from the group consisting of amino acid 15 to 31 of beta-sheet I, amino acid 43 to 61 of beta-sheet I, amino acid 87 to 104 of the loop and beta-sheet III, amino acid 133 to 163 of the alpha-helix and surrounding loops, and amino acid 177 to 185 of beta-sheet I, based on the amino acid numbering from *B. circulans* xylanase.
10. The modified xylanase of Claim 9, wherein the cysteine amino acid is located at amino acid position 179, based on the amino acid numbering from *B. circulans* xylanase.
11. A modified family G xylanase of Claim 1, wherein the N-terminal to C-terminal disulfide bond results from an extension at the N-terminus and C-terminus end of the protein to add cysteine or by the conversion of amino acids at the termini to cysteine.
12. The modified family G xylanase of Claim 11, wherein the N-terminus is extended by adding a glycine at position -1, the C-terminus is extended by adding glycine and cysteine at position 186 and 187, respectively and wherein the alanine at position 187 is converted into cysteine.
13. The modified xylanase of Claim 1, wherein the xylanase is modified at the N-terminus by combining a mutation selected from the group consisting of: the introduction of tyrosine at amino acid position 8, the introduction of phenylalanine at amino acid position 8, the introduction of proline at amino acid position 22, and the introduction of an N-terminal to C-terminal disulfide bridge, with a mutation at position 3 or 4.
14. The modified xylanase of Claim 1, wherein said modified xylanase are produced from clones selected from the group consisting of TS1, TS2, TS3, TS3a, TS5a, TS6a, TS7a, TS10a, TS14a, TS15a, TS17a, TS19a, TS20a and TS21a.

15. The modified xylanase of Claim 14, wherein said modified xylanase are produced from clones selected from the group consisting of TS3, TS3a, TS5a, TS6a, TS7a, TS10a, TS14a, TS15a, TS17a, TS19a, TS20a and TS21a.

16. The modified xylanase of Claim 15, wherein said modified xylanase are produced from clones selected from the group consisting of TS6a, TS14a, TS17a, TS19a and TS21a.

17. A modified family G xylanase essentially having the structure of the *B. circulans* enzyme or mutated to essentially have this structure, wherein said xylanase has increased stability and wherein said xylanase is modified through either the introduction of at least one non-native disulfide bridge, the introduction of at least one N-terminal mutation, or combinations thereof; and wherein said modified xylanase is produced from clones selected from the group consisting of TS1, TS2, TS3, TS3a, TS5a, TS6a, TS7a, TS10a, TS14a, TS15a, TS17a, TS19a, TS20a and TS21a.

18. A modified family G xylanase essentially having the structure of the *B. circulans* enzyme or mutated to essentially have this structure, wherein said xylanase has increased stability and wherein said xylanase is modified through either the introduction of at least one non-native disulfide bridge, the introduction of at least one N-terminal mutation, or combinations thereof; and wherein said modified xylanase is produced from clones selected from the group consisting of TS6a, TS14a, TS17a, TS19a and TS21a.

BP	1	RTITNNEMGN	HSGYDYELWK	DYGNT-SMTL	NNGGAFSAGW	N--NIGNA	45
CA	32	KTITSNEIGV	NGGYDYELWK	DYGNT-SMTL	KNGGAFSCQW	S--NIGNA	76
RF	1	SAADQQTRGN	VGGYDYEMWN	QNGQGQASMN	PGAGSFTCSW	S--NIENF	46
TR2	1	QTIQPGTGY	NNGYFYSYWN	DGHGGVITYN	GPGGQFSVNW	S--NSGNF	45
TV	1	QTIQPGTGY	NNGYFYSYWN	DGHGGVITYN	GPGGQFSVNW	S--NSGNF	45
TH	1	QTIQPGTGY	SNGYYSYWN	DGHAGVITYN	GGGGSFTVNW	S--NSGNF	45
SC	1	SGTPSSTGT	DGGYYSWWT	DGAGDATYQN	NGGGSYTLTW	SG--NNGNL	46
AN	1	S	AGINYVQNYN	GNLGDFTY-D	ESAGTFSMYW	EDGVSSDF	37
AT	1		AGINYVQNYN	QNLGDFTY-D	ESAGTFSMYW	EDGVSSDF	37
TR1	1		ASINYDQNYQ	TGG-QVSY-	PSNTGFSVNW	N--TQDDF	34
SS	1	ATTIT-NETGY	D-GMYYSFWT	DGGGSVSMTL	NGGGSYSTRW	T--NCGNF	45
SLB	1	DTVVTNQEGT	NNGYYSFWT	DSQGTVMNM	GSGGQYSTSW	R--NTGNF	47
SLC	1	ATTITTNTGT	D-GMYYSFWT	DGGGSVSMTL	NGGGSYSTRW	T--NCGNF	46
BC	1		ASTDYWQNW	DGGGIVNAV	GSGGNYSVNW	S--NTGNF	36
BS	1		ASTDYWQNW	DGGGIVNAV	GSGGNYSVNW	S--NTGNF	36

ConsensusG. ..GYYY..W. DGGG.V.... ..GG.FS..W S..N.GNF

BP	46	LFRK-GKKFD	ST-RTHQLG	NISINYNASF	N-PSGNSYLC	VYGWTQSP	90
CA	77	LFRK-GKKFN	DT-QTYKQLG	NISVNYDCNY	Q-PYGNSYLC	VYGWTSSP	121
RF	47	LARM-GKNYD	SQKKNYKAFG	NIVLTYDVEY	T-PRGNSYMC	VYGWTRNP	92
TR2	46	VGGK-GWQPG	TKNKV-----	---INFS-GS	YNPNNGNSYLS	VYGWSRNP	83
TV	46	VGGK-GWQPG	TKNKV-----	---INFS-GS	YNPNNGNSYLS	VYGWSRNP	83
TH	46	VGGK-GWQPG	TKNKV-----	---INFS-GS	YNPNNGNSYLS	IYGWSRNP	83
SC	47	VGGK-GWNPG	AASRS-----	---ISYS-GT	YQPNNGNSYLS	VYGWTRSS	84
AN	38	VVGL-GWTTG	SSNA-----	---ITYSAEY	SASGSSSYLA	VYGWVNYP	76
AT	38	VVGLGGWTTG	SSNA-----	---ITYSAEY	SASGSASYLA	VYGWVNYP	76
TR1	35	VVGW-GWTTG	SSAP-----	---INFGGSF	SVNSGTGLLS	VYGWSTNP	72
SS	46	VAGK-GWANG	GR-RT-----	---VRYT-GW	FNPSGNGYGC	LYGWTSNP	82
SLB	48	VAGK-GWANG	GR-RT-----	---VQYS-GS	FNPSGNAYLA	LYGWTSNP	84
SLC	47	VAGK-GWSTG	DGN-----	---VRYN-GY	FNPVGNGYGC	LYGWTSNP	82
BC	37	VVGK-GWTTG	SPFRT-----	---INYNAGV	WAPNGNGYLT	LYGWTRSP	75
BS	37	VVGK-GWTTG	SPFRT-----	---INYNAGV	WAPNGNGYLT	LYGWTRSP	75

Consensus V.GK.GW..GINY..G. ..P.GNSYL. VYGWT.NP

BP	91	LAEYYIVDSW	GTYR-PT--G	AYKGSFYADG	GTYDIYETTR	VNQPSIIG	135
CA	122	LVEYYIVDSW	GSWRPP--GG	TSKGTITVDG	GIYDIYETTR	INQPSIQG	167
RF	93	LMEYYIVEGW	GDWRPPGNDG	EVKGTVSANG	NTYDIRKTMR	YNQPSLDG	140
TR2	84	LIEYYIVENF	GTYN-PSTGA	TKLGEVTSBG	SVYDIYRTQR	VNQPSIIG	130
TV	84	LIEYYIVENF	GTYN-PSTGA	TKLGEVTSBG	SVYDIYRTQR	VNQPSIIG	130
TH	84	LIEYYIVENF	GTYN-PSTGA	TKLGEVTSBG	SVYDIYRTQR	VNQPSIIG	130
SC	85	LIEYYIVESY	GSYD-PSSAA	SHKGSVTCNG	ATYDILSTWR	YNAPSIDG	131
AN	77	GAEYYIVEDY	GDYN-PCSSA	TSLGTVYSDG	STYQVCTDTR	INEPSITG	123
AT	77	QAEYYIVEDY	GDYN-PCSSA	TSLGTVYSDG	STYQVCTDTR	INEPSITG	123
TR1	73	LVEYYIMEDN	HNY--PAQ-G	TVKGTVTSBG	ATYTIWENTR	VNEPSIQG	117
SS	83	LVEYYIVDNW	GSYR-PT--G	ETRGTVHSDG	GTYDIYKTTR	YNAPSVEA	127
SLB	85	LVEYYIVDNW	GTYR-PT--G	EYKGTVTSBG	GTYDIYKTTR	VNKPSVEG	129
SLC	83	LVEYYIVDNW	GSYR-PT--G	TYKGTVSSDG	GTYDIYQTTR	YNAPSVEG	127
BC	76	LIEYYVVDWS	GTYR-PT--G	TYKGTVKS DG	GTYDIYTTTR	YNAPSIDG	120
BS	76	LIEYYVVDWS	GTYR-PT--G	TYKGTVKS DG	GTYDIYTTTR	YNAPSIDG	120

Consensus L.EYYIVE.W G.YR.P...G T.KGTV.SDG .TYDIY.TTR .N.PSI.G

FIGURE 1

BP	136	-IATFKQYWS	VRQTKRTS--	-----GTVS	VSAHFRKWES	LGMPM-GK	174
CA	168	-NTTFKQYWS	VRRTKRTS--	-----GTIS	VSKHFAAWES	KGMP-L-GK	206
RF	141	-TATFPQYWS	VRQTS GSANN	QTNYMKGTID	VSKHFD AWSA	AGLDMSGT	187
TR2	131	-TATFYQYWS	VRRNHR-S-S	-----GSVN	TANHFN AWAQ	QGLTL-GT	169
TV	131	-TATFYQYWS	VRRTHR-S-S	-----GSVN	TANHFN AWAQ	QGLTL-GT	169
TH	131	-TATFYQYWS	VRRNHR-S-S	-----GSVN	TANHFN AWAQ	QGLTL-GT	169
SC	132	-TQTFEQFWS	VRNPKKAPGG	SIS---GTV	VQCHFD AWKG	LG MNLGSE	175
AN	124	-TSTFTQYFS	VRESTRTS--	-----GTVT	VANHFNF WAQ	HGFGN-SD	162
AT	124	-TSTFTQYFS	VRESTRTS--	-----GTVT	VANHFNF WAH	HGFGN-SD	162
TR1	118	-TATFNQYIS	VRNSPR-T-S	-----GTVT	VQNHFN-WAS	LGLHLGQM	155
SS	128	-PAAFDQYWS	VRQSKVT--S	-----GTIT	TGNHFD AWAR	AGMNMGNF	168
SLB	130	TR-TFDQYWS	VRQSKR-TG-	-----GTIT	TGNHFD AWAR	AGMPLGNF	168
SLC	128	TK-TFQQYWS	VRQSKVTS GS	-----GTIT	TGNHFD AWAR	AGMNMGQF	168
BC	121	DRTTFTQYWS	VRQSKRPTGS	N-----ATIT	FTNHVN AWKS	HGMNLGSN	163
BS	121	DRTTFTQYWS	VRQSKRPTGS	N-----ATIT	FSNHVN AWKS	HGMNLGSN	163

Consensus .T.TF.QYWS VR.SKR.S..GTVT ..NHFN AWA. .GH.L...

BP	175	MYETAFTVEG	YQSSGSANVM	TNQLFIGN		201
CA	207	MHETAFNIEG	YQSSGKADVN	SMSINIGK		233
RF	188	LYEVSLNIEG	YRSNGSANVK	SVSV		211
TR2	170	MDYQIVAVEG	YFSSGSASI-	TVS		190
TV	170	MDYQIVAVEG	YFSSGSASI-	TVS		190
TH	170	MDYQIVAVEG	YFSSGSASI-	TVS		190
SC	176	HNYQIVATEG	YQSSGTATI-	TVT		197
AN	163	FNYQVM AVEA	WSGAGSASV-	TISS		184
AT	163	FNYQVVAVEA	WSGAGSAAV-	TISS		184
TR1	157	MNYQVVAVEG	WGGSGSASQ-	SVSN		178
SS	167	RYYMIMATEG	YQSSGSSTI-	TVSG		189
SLB	169	SYYMIMATEG	YQSSGTSSI-	NVGGTGGGDS	GGATTGAVAA	215
SLC	169	RYYMIMATEG	YQSSGSSNI-	TVSG		191
BC	164	WAYQVM ATEG	YQSSGSSNV-	TVW		185
BS	164	WAYQVM ATEG	YQSSGSSNV-	TVW		185

Consensus ..YQ..A.EG YQSSGSA... TVS

BP	<i>Bacillus pumilus</i>
CA	<i>Clostridium acetobutylicum</i> , Xyn B
RF	<i>Ruminococcus flavefaciens</i>
TR2	<i>Trichoderma reesei</i> , XYN II, 21kD, pI 9.0
TV	<i>Trichoderma viride</i> , 20kD
TH	<i>Trichoderma harzianum</i> , 20kD
SC	<i>Schizophyllum commune</i> , Xylanase A
AN	<i>Aspergillus niger</i> , var. awamori
AT	<i>Aspergillus tubigenensis</i> , A
TR1	<i>Trichoderma reesei</i> , XYN I, 19kD, pI 5.2
BS	<i>Bacillus subtilis</i>
BC	<i>Bacillus circulans</i>
SLB	<i>Streptomyces lividans</i> , Xln B
SLC	<i>Streptomyces lividans</i> , Xln C
SS	<i>Streptomyces</i> sp. #36a

FIGURE 1 CONT'D

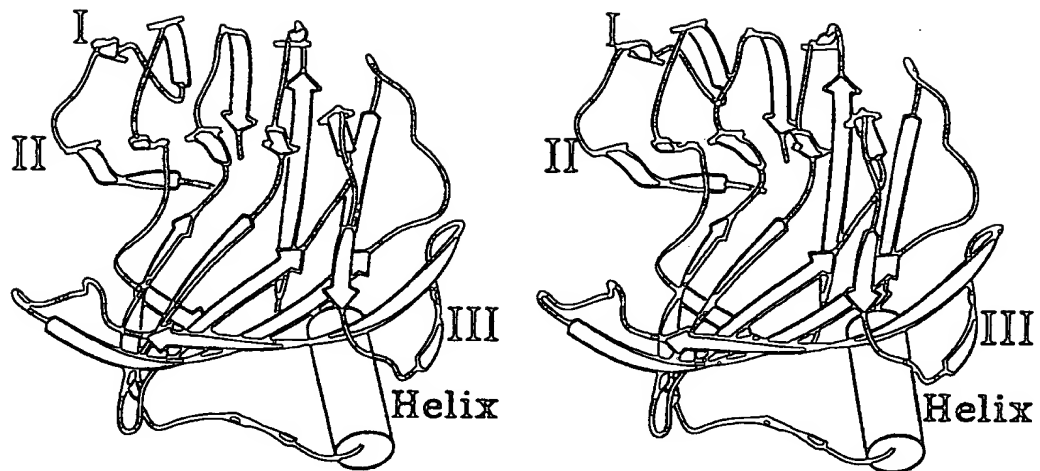


FIGURE 2

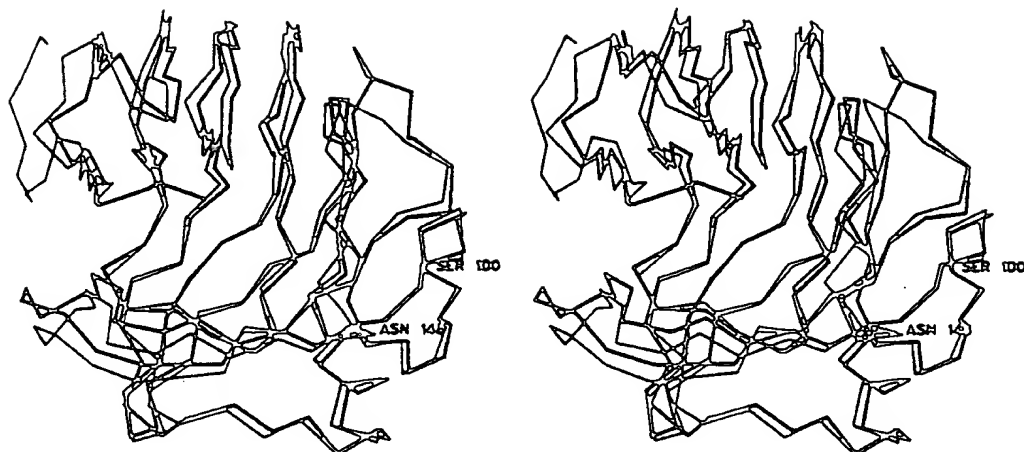


FIGURE 3

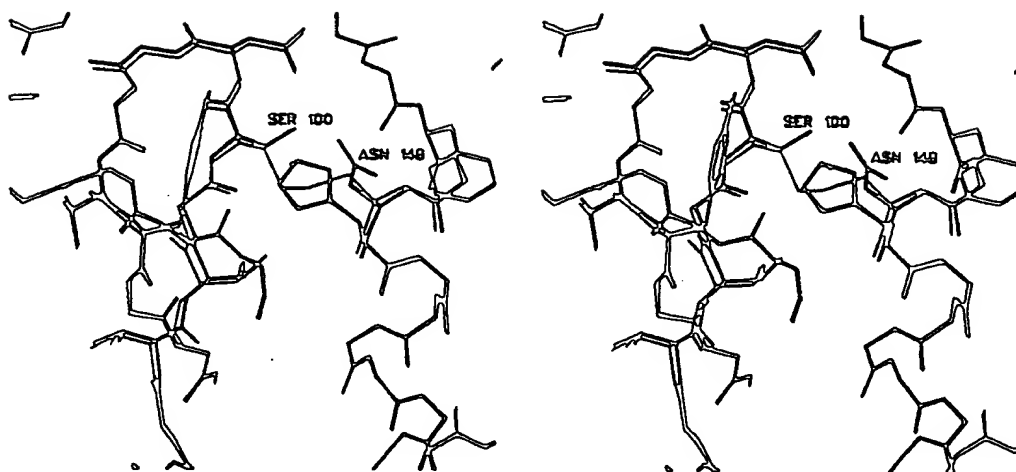
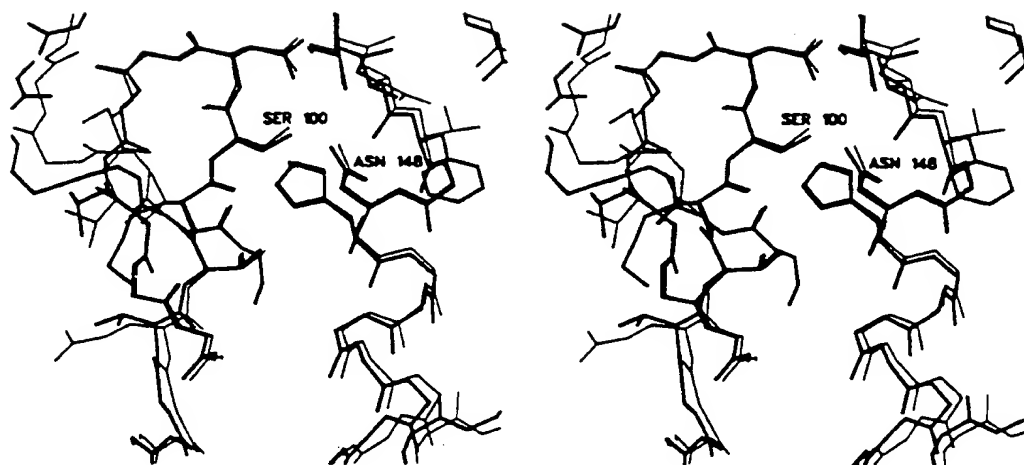


FIGURE 4

**FIGURE 5**

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
A	S	T	D	Y	W	Q	N	W	T	D	G	G	G	I	V
<u>GCT AGC</u>	ACA	GAC	TAC	TGG	CAA	AAT	TGG	ACT	GAT	GGG	GGC	GGT	ATA	GTA	
<u>CGA TCG</u>	TGT	CTG	ATG	ACC	GTT	TTA	ACC	TGA	CTA	CCC	CCG	CCA	TAT	CAT	
NheI 5' PCR primer site															
17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
N	A	V	N	G	S	G	G	N	Y	S	V	N	W	S	N
AAC	GCT	GTC	AAT	GGG	TCT	GGC	GGG	AAT	TAC	AGT	GTT	AAT	TGG	TCT	AAT
TTG	CGA	CAG	TTA	CCC	AGA	CCG	CCC	TTA	ATG	TCA	CAA	TTA	ACC	AGA	TTA
33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
T	G	N	F	V	V	G	K	G	W	T	T	G	S	P	F
ACC	GGA	AAT	TTT	GTT	GTT	GGT	AAA	GGT	TGG	ACT	ACA	GGT	TCG	CCA	TTT
TGG	CCT	TTA	AAA	CAA	CAA	CCA	TTT	CCA	ACC	TGA	TGT	CCA	AGC	GGT	AAA
49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64
R	T	I	N	Y	N	A	G	V	W	A	P	N	G	N	G
AGG	ACG	ATA	AAC	TAT	AAT	GCC	GGA	GTT	TGG	<u>GCG CCG</u>	AAT	GGC	AAT	GGA	
TCC	TGC	TAT	TTG	ATA	TTA	CGG	CCT	CAA	ACC	<u>CGC GGC</u>	TTA	CCG	TTA	CCT	
NaeI															
65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
Y	L	T	L	Y	G	W	T	R	S	P	L	I	E	Y	Y
TAT	TTA	ACT	TTA	TAT	GGT	TGG	ACG	AGA	TCA	CCT	CTC	ATA	<u>GAA TAT TAT</u>		
ATA	AAT	TGA	AAT	ATA	CCA	ACC	TGC	TCT	AGT	GGA	GAG	TAT	CTT	ATA	ATA
SspI															
81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96
V	V	D	S	W	G	T	Y	R	P	T	G	T	Y	K	G
GTA	GTG	GAT	TCA	TGG	GGT	ACT	TAT	AGA	CCT	ACT	GGA	ACG	TAT	AAA	GGT
CAT	CAC	CTA	AGT	ACC	CCA	TGA	ATA	TCT	GGA	TGA	CCT	TGC	ATA	TTT	<u>CCA</u>
97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112
T	V	K	S	D	G	G	T	Y	D	I	Y	T	T	T	R
ACT	GTA	AAA	AGT	GAT	GGG	GGT	<u>ACA TAT GAC</u>	ATA	TAT	ACA	ACT	ACA	CGT		
<u>TGA CAT TTT TCA CTA CCC CCA</u>	TGT	ATG	CTG	TAC	ATA	TGT	TGC	TGT	GCA						
S100C mutagenic primer site NdeI															
113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128
Y	N	A	P	S	I	D	G	D	R	T	T	F	T	Q	Y
TAT	AAC	GCA	CCT	TCC	ATT	GAT	<u>GGC GAT GGC</u>	ACT	ACT	TTT	ACG	CAG	TAC		
ATA	TTG	CGT	GGA	AGG	TAA	CTA	CCG	CTA	GCG	TGA	TGA	AAA	TGC	GTC	ATG
PvuI															
129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144
W	S	V	R	Q	S	K	R	P	T	G	S	N	A	T	I
TGG	AGT	GTT	CGC	CAG	TCG	AAG	AGA	CCA	ACC	GGA	AGC	AAC	GCT	ACA	ATC
ACC	TCA	CAA	GCG	GTC	AGC	TTC	TCT	GGT	TGA	CCA	TCG	TTG	CGA	TGT	TAG

FIGURE 6

145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160
 T F S N H V N A W K S H G M N L
 ACT TTC AGC AAT CAT GTG AAC GCA TGG AAG AGC CAT GGA ATG AAT CTG
 TGA AAG TCG TTA GTA CAC TTG CGT ACC TTC TCG GTA CCT TAC TTA GAT
 NcoI

161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176
 G S N W A Y Q V M A T E G Y Q S
 GGC AGT AAT TGG GCT TAC CAA GTC ATG GCG ACA GAA GGA TAT CAA AGT
 CCG TCA TTA ACC CGA ATG GTT CAT TAC CGC TGT CTT CCT ATA GAT TCA
 EcoRV

177 178 179 180 181 182 183 184 185 STOP
 S G S S N V T V W
 AGT GGA AGT TCT AAC GTA ACA GTG TGG TAA CAGATCATCC TTAATCAGGG
 TCA CCT TCA AGA TTG CAT TGT CAC ACC ATT GTCTAGTAGG AATTAGTCCC

GTAGCTAACG GGCTGCTGAT CGTTCCTTGA GAAGTTTGA TAATCAATGA TTATTAAAT
 CATCGATTGC CCGACGACTA GCAAGGAACT CTTCAAAAT ATTAGTTACT AATAATTTTA
 3' PCR primer

CGTTAGTAA TGGTTAAAGG TTGTTTTCTA CTAGGTGAAC GGCCTTGGAA TTGCTGGAGG
GCAATCATT ACCAATTTCC AACAAAAGAT GATCCACTTG CCGGAACCTT AACGACCTCC
 binding site

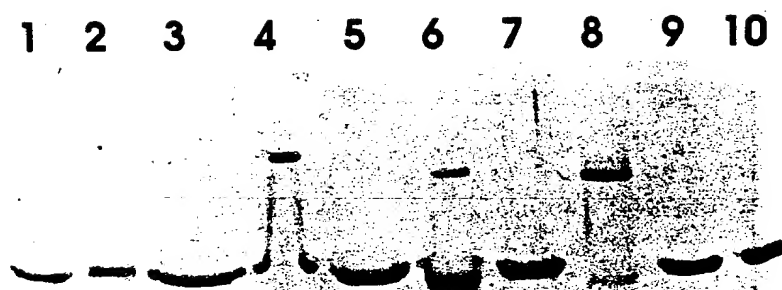
TAGGGTATTC TCCATCTGGT TTTT
 ATCCCATAAG AGGTAGACCA AAAA

FIGURE 6 CONT'D

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
A	S	T	D	Y	W	Q	N	W	T	D	G	G	G	I	V
GCT	AGC	ACA	GAC	TAC	TGG	CAA	AAT	TGG	ACT	GAT	GGG	GGC	GGT	ATA	GTA
CGA	TCG	TGT	CTG	ATG	ACC	GTT	TTA	ACC	TGA	CTA	CCC	CCG	CCA	TAT	CAT
NheI															
17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
N	A	V	N	G	S	G	G	N	Y	S	V	N	W	S	N
AAC	GCT	GTC	AAT	GGG	TCT	GGC	GGG	AAT	TAC	AGT	GTT	AAT	TGG	TCT	AAT
TTG	CGA	CAG	TTA	CCC	AGA	CCG	CCC	TTA	ATG	TCA	CAA	TTA	ACC	AGA	TTA
33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
T	G	N	F	V	V	G	K	G	W	T	T	G	S	P	F
ACC	GGA	AAT	TTT	GTT	GTT	GGT	AAA	GGT	TGG	ACT	ACA	GGT	TCG	CCA	TTT
TGG	CCT	TTA	AAA	CAA	CAA	CCA	TTT	CCA	ACC	TGA	TGT	CCA	AGC	GGT	AAA
49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64
R	T	I	N	Y	N	A	G	V	W	A	P	N	G	N	G
AGG	ACG	ATA	AAC	TAT	AAT	GCC	GGA	GTT	TGG	GGG	CCG	AAT	GGC	AAT	GGA
TCC	TGC	TAT	TTG	ATA	TTA	CGG	CCT	CAA	ACC	CGC	GGC	TTA	CCG	TTA	CCT
NaeI															
65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
Y	L	T	L	Y	G	W	T	R	S	P	L	I	E	Y	Y
TAT	TTA	ACT	TTA	TAT	GGT	TGG	ACG	AGA	TCA	CCT	CTC	ATA	GAA	TAT	TAT
ATA	AAT	TGA	AAT	ATA	CCA	ACC	TGC	TCT	AGT	GGA	GAG	TAT	CTT	ATA	ATA
SspI															
81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96
V	V	D	S	W	G	T	Y	R	P	T	G	T	Y	K	G
GTA	GTG	GAT	TCA	TGG	GGT	ACT	TAT	AGA	CCT	ACT	GGA	ACG	TAT	AAA	GGT
CAT	CAC	CTA	AGT	ACC	CCA	TGA	ATA	TCT	GGA	TGA	CCT	TGC	ATA	TTT	CCA
97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112
T	V	K	S	D	G	G	T	Y	D	I	Y	T	T	T	R
ACT	GTA	AAA	AGT	GAT	GGG	GGT	ACA	TAT	GAC	ATC	TAC	ACC	ACC	ACA	AGA
TGA	CAT	TTT	TCA	CTA	CCC	CCA	TGT	ATG	CTG	TAG	ATG	TGG	TGG	TGT	TCT
NdeI															
V908C mutagenic primer site															
113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128
Y	N	A	P	S	I	D	G	D	R	T	T	F	T	Q	Y
TAC	AAC	GCA	CCT	TCC	ATC	GAT	GGC	GAT	CGG	ACC	ACC	TTT	ACT	CAG	TAC
ATG	TTG	CGT	GGA	AGG	TAG	CTA	CCG	CTA	GCC	TGG	TGG	AAA	TGA	GTC	ATG
ClaI															
PvuI															
129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144
W	S	V	R	Q	S	K	R	P	T	G	S	N	A	T	I
TGG	AGT	GTT	AGA	CAA	TCT	AAG	CGG	CCG	ACT	GGT	TCG	AAC	GCC	ACC	ATT
ACC	TCA	CAA	TCT	GTT	AGA	TTC	GCC	GGG	TGA	CCA	AGC	TTG	CGG	TGG	TAA
EagI/EaeI															
BstBI															

FIGURE 7

FIGURE 7 CONT'D

**FIGURE 8**

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
A	S	T	D	Y	W	Q	N	W	T	D	G	G	G	I	V
<u>GCT AGC</u>	ACA	GAT	TAC	TGG	CAA	AAC	TGG	ACA	GAC	GGT	GGC	GGT	ATC	GTT	
<u>CGA TCG</u>	TGT	CTA	ATG	ACC	GTT	TTG	ACC	TGT	CTG	CCA	CCG	CCA	TAG	CAA	
NheI															
17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
N	A	V	N	G	S	G	G	N	Y	S	V	N	W	S	N
AAT	GCC	GTG	AAC	GGC	<u>TCC GGA</u>	GGC	AAC	TAC	AGC	GTG	AAT	TGG	TCT	AAT	
TTA	CGG	CAC	TTG	CCG	<u>AGG CCT</u>	CCG	TTG	ATG	TCG	CAC	TTA	ACC	AGA	TTA	
BspEI															
33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
T	G	N	F	V	V	G	K	G	W	T	T	G	S	P	F
ACT	GGG	AAC	TTC	GTA	GTC	GGA	AAA	GGT	TGG	ACG	ACA	<u>GGA TCC</u>	CCG	TTC	
TGA	CCC	TTG	AAG	CAT	CAG	CCT	TTT	CCA	ACC	TGC	TGT	<u>CCT AGG</u>	GGC	AAG	
BamHI															
49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64
R	T	I	N	Y	N	A	G	V	W	A	P	N	G	N	G
<u>CGT ACG</u>	ATC	AAC	TAC	AAC	GCT	GGC	GTT	<u>TGG GCC</u>	CCG	AAT	GGT	AAC	GGT		
<u>GCA TGC</u>	TAG	TTG	ATG	TTG	CGA	CCG	CAA	ACC	<u>CGG GGC</u>	TTA	CCA	TTG	CCA		
SplI Apal															
65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
Y	L	T	L	Y	G	W	T	R	S	P	L	I	E	Y	Y
TAC	CTG	ACA	CTG	TAT	GGC	TGG	<u>ACG CGT</u>	TCG	CCA	CTG	ATT	<u>GAA TAT</u>	TAC		
ATG	GAC	TGT	GAC	ATA	CCG	ACC	<u>TGC GCA</u>	AGC	GGT	GAC	TAA	<u>CTT ATA</u>	ATG		
MluI SspI															
81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96
V	V	D	S	W	G	T	Y	R	P	T	G	T	Y	K	G
GTT	<u>GTC GAC</u>	TCT	TGG	GGA	ACG	TAC	CGT	CCG	ACT	GGA	ACC	TAC	AAA	GGC	
CAA	<u>CAG CTG</u>	AGA	ACC	CCT	TGC	ATG	GCA	GGC	TGA	CCT	TGG	ATG	TTT	CCG	
Sall															
97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112
T	V	K	S	D	G	G	T	Y	D	I	Y	T	T	T	R
ACA	GTC	AAA	AGC	GAT	GGT	<u>GGT ACC</u>	TAC	GAC	ATC	TAC	ACC	ACC	ACA	AGA	
TGT	CAG	TTT	TCG	CTA	CCA	<u>CCA TGG</u>	ATG	CTG	TAG	ATG	TGG	TGG	TGT	TCT	
KpnI															
113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128
Y	N	A	P	S	I	D	G	D	R	T	T	F	T	Q	Y
TAC	AAC	GCA	CCT	TCC	<u>ATC GAT</u>	GGC	<u>GAT CGG</u>	ACC	ACC	TTT	ACT	CAG	TAC		
ATG	TTG	CGT	GGA	AGG	<u>TAG CTA</u>	CCG	<u>CTA GCC</u>	TGG	TGG	AAA	TGA	GTC	ATG		
ClaI PvuI															

FIGURE 9

```

177 178 179 180 181 182 183 184 185 STOP
  S   G   S   S   N   V   T   V   W
TCT GGT TCT TCC AAC GTT ACA GTG TGG TAA AGATCTTGAAGCTT
AGA CCA AGA AGG TTG CAA TGT CAC ACC ATT TCTAGAACTTCGAA
SacI                                     BglII      HindIII

```

BN8DOCID: <WO 9424270A2 1>



1 2 3 4 5 6 7

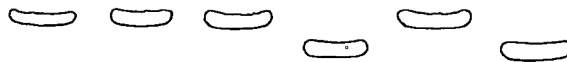


FIGURE 10

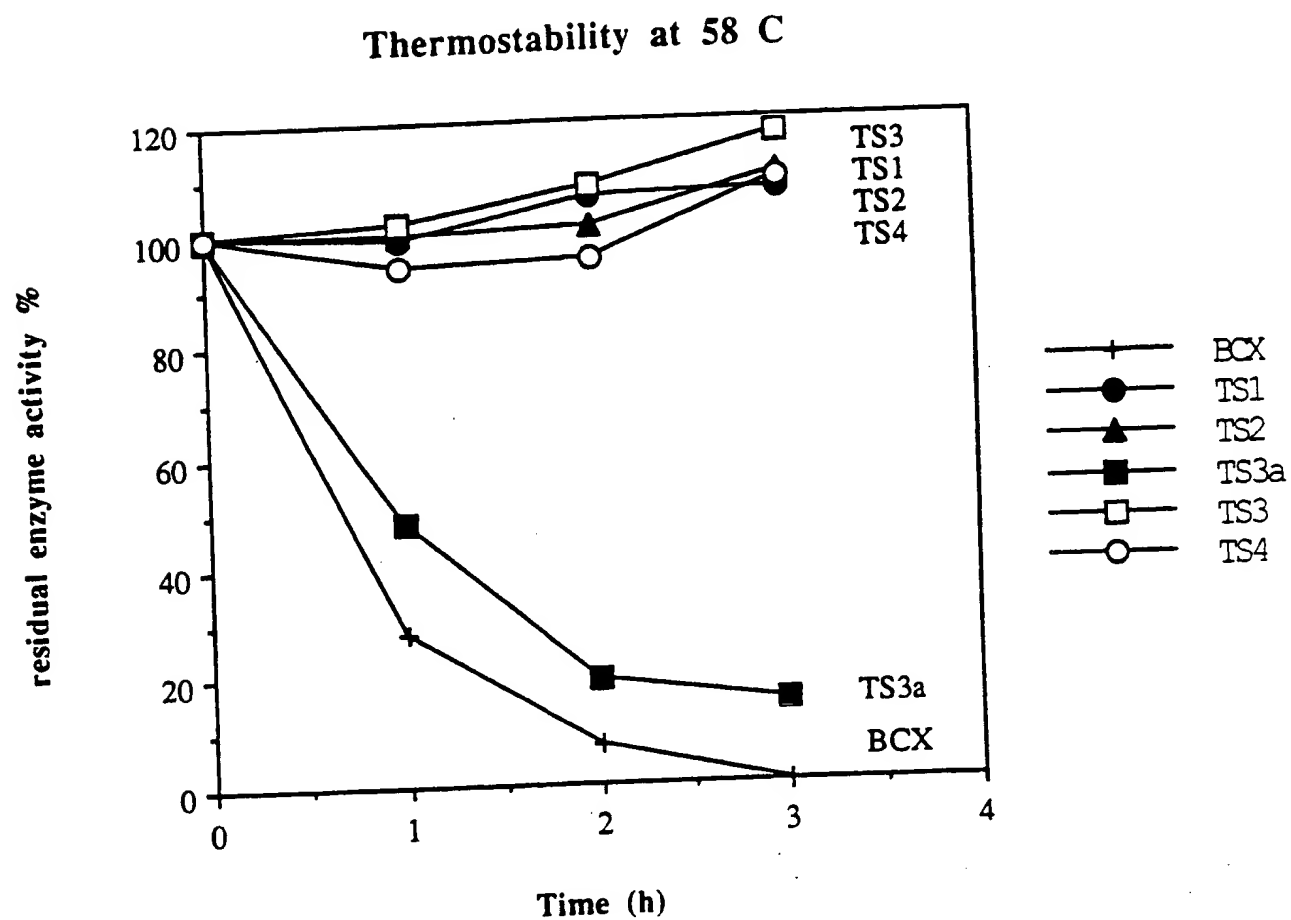
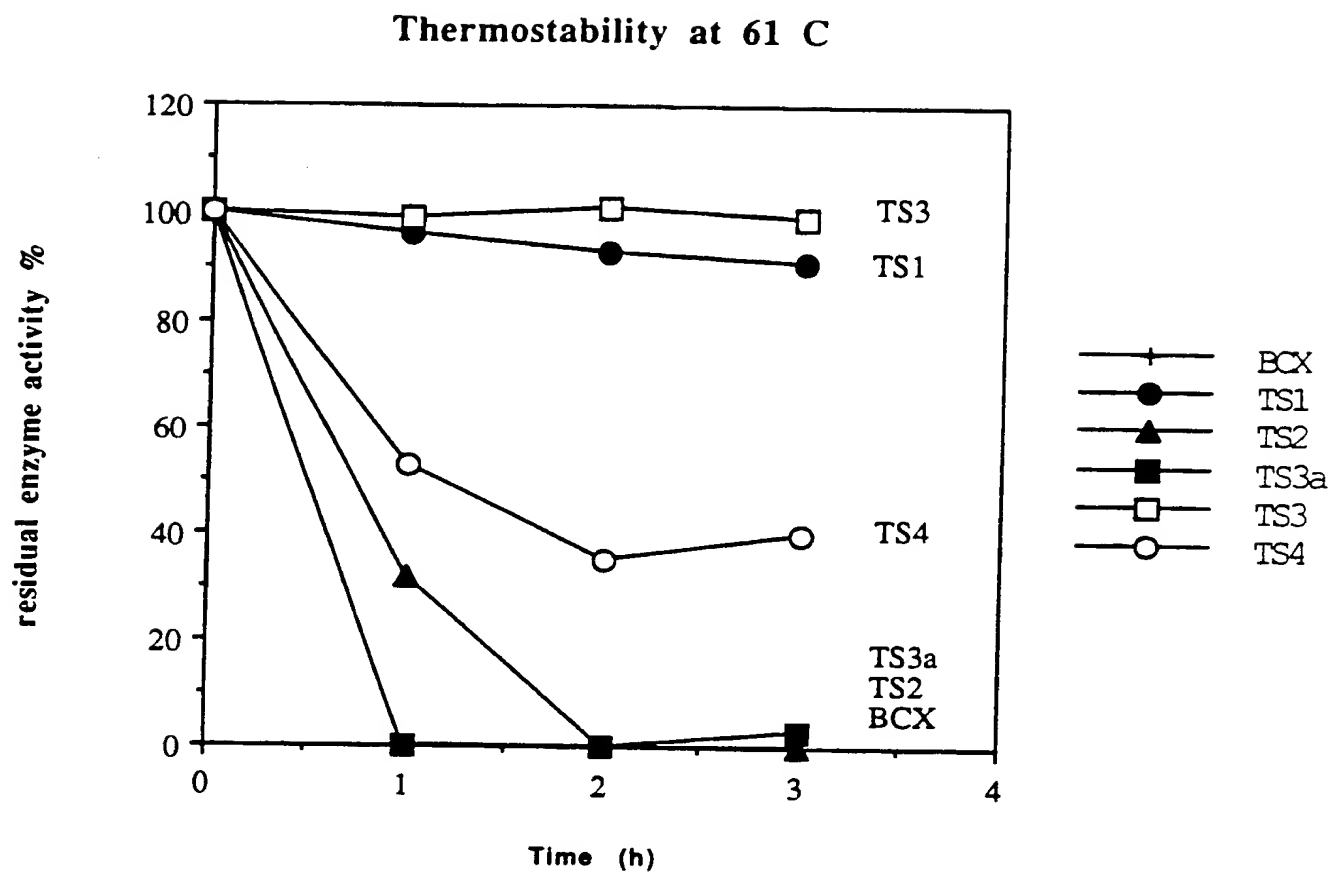


FIGURE 11

**FIGURE 12**

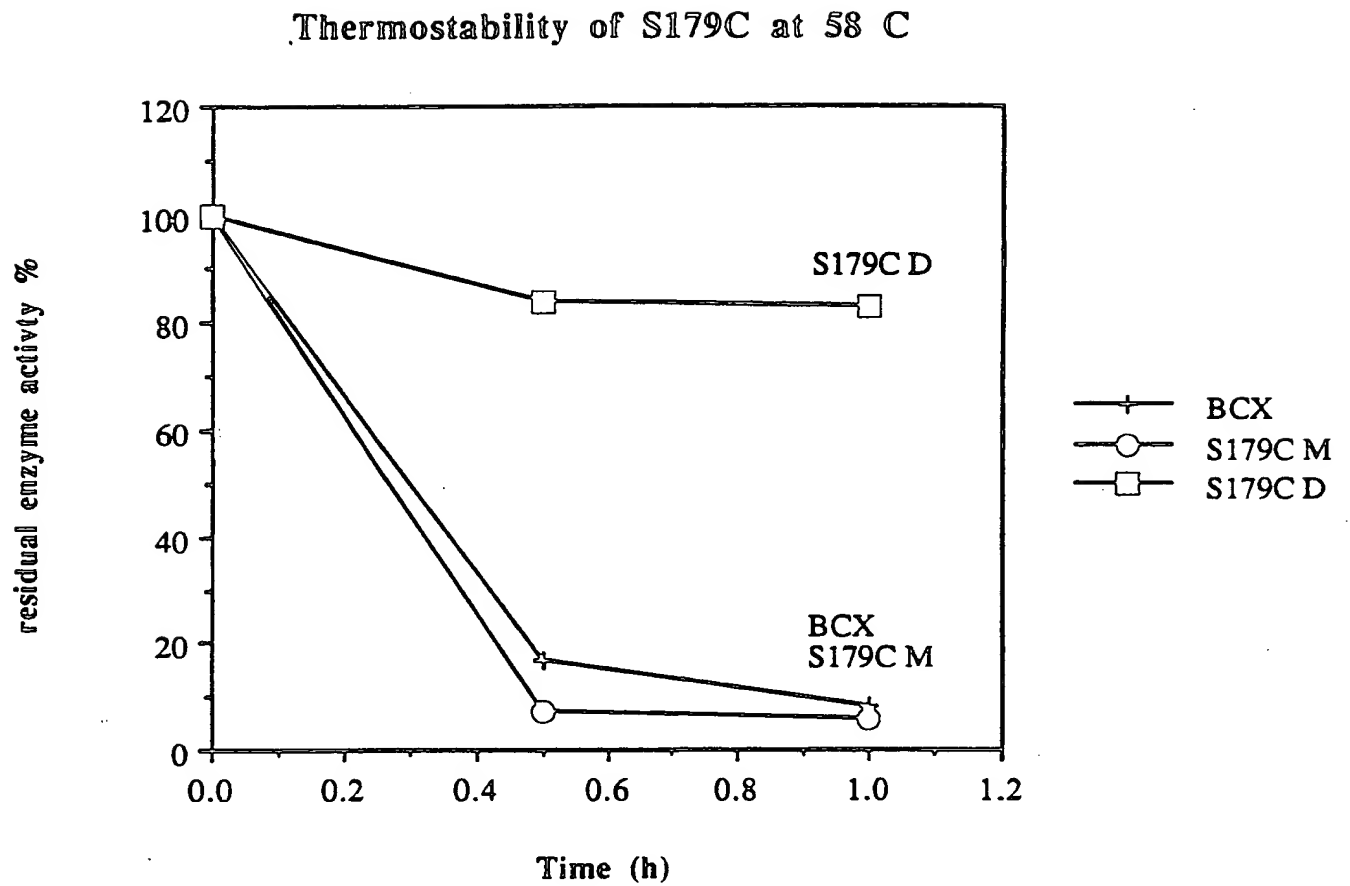
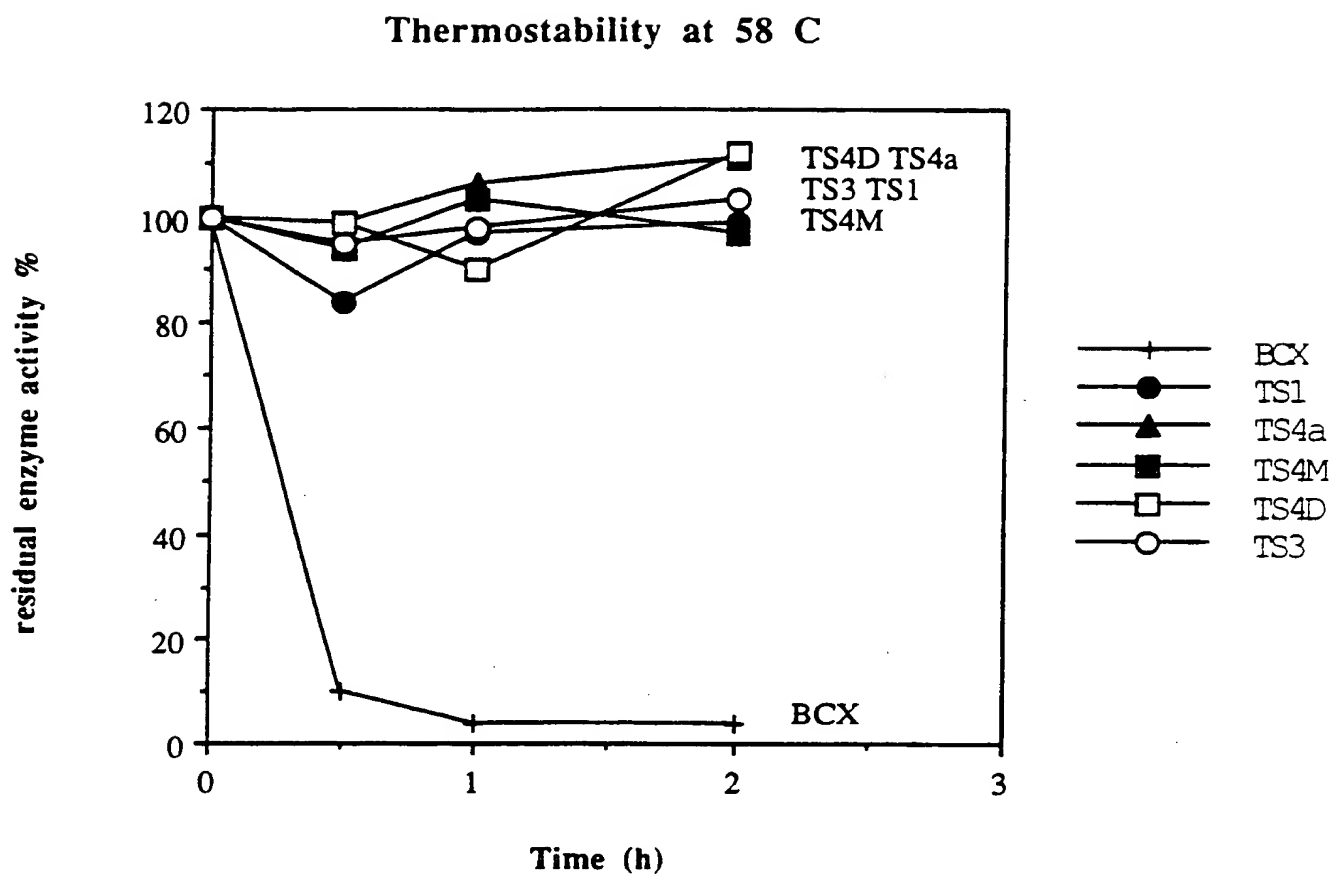


FIGURE 13

**FIGURE 14**

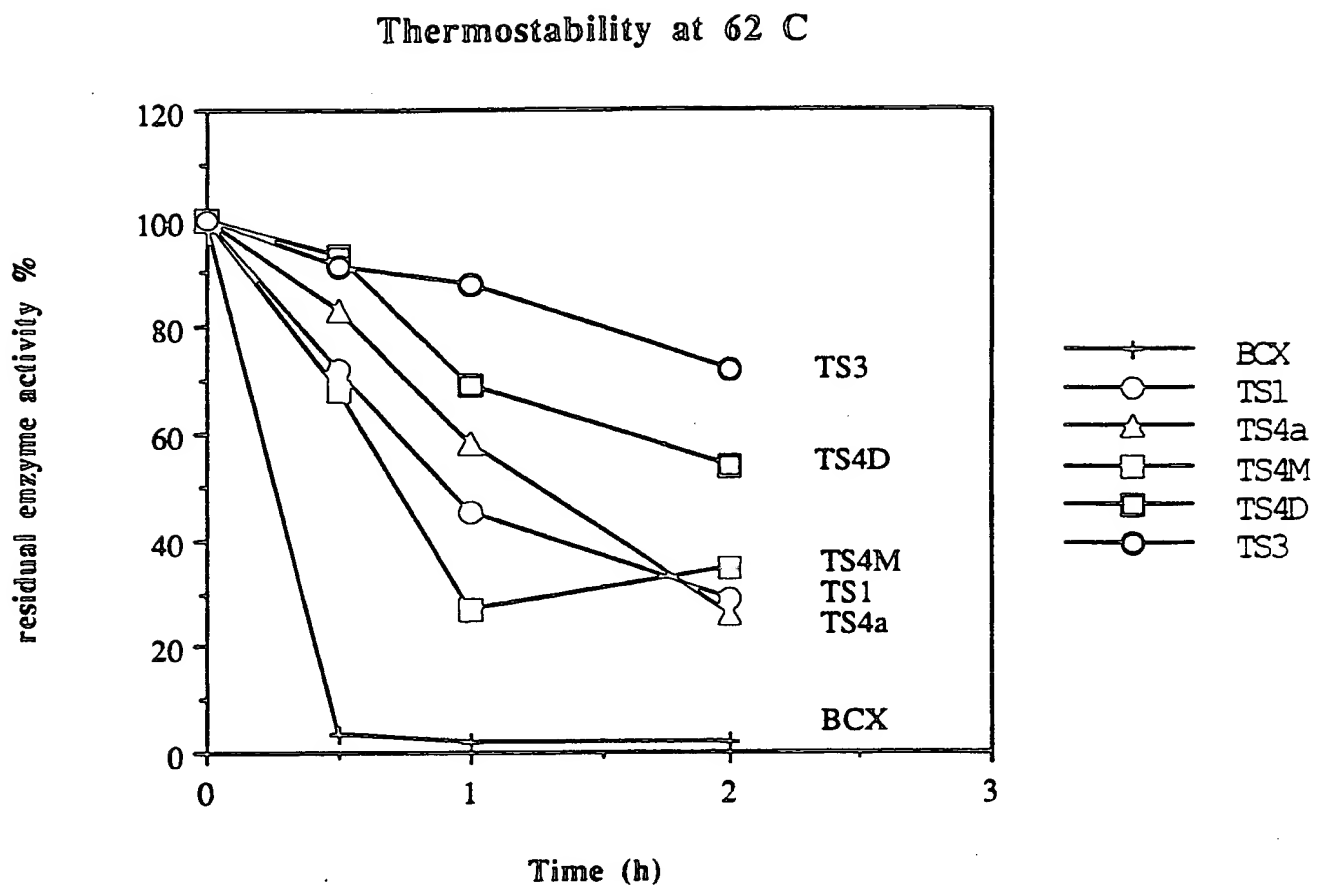
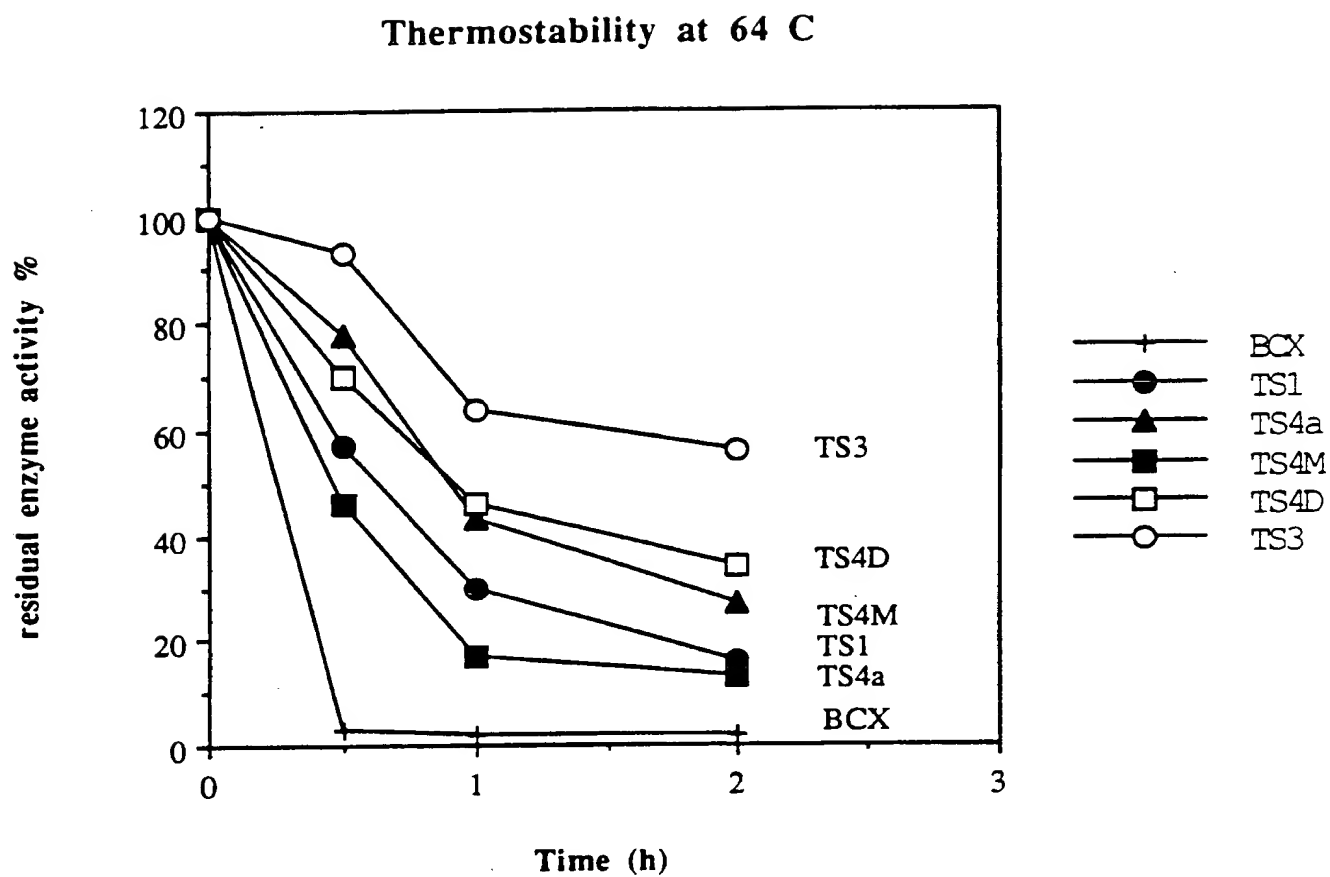
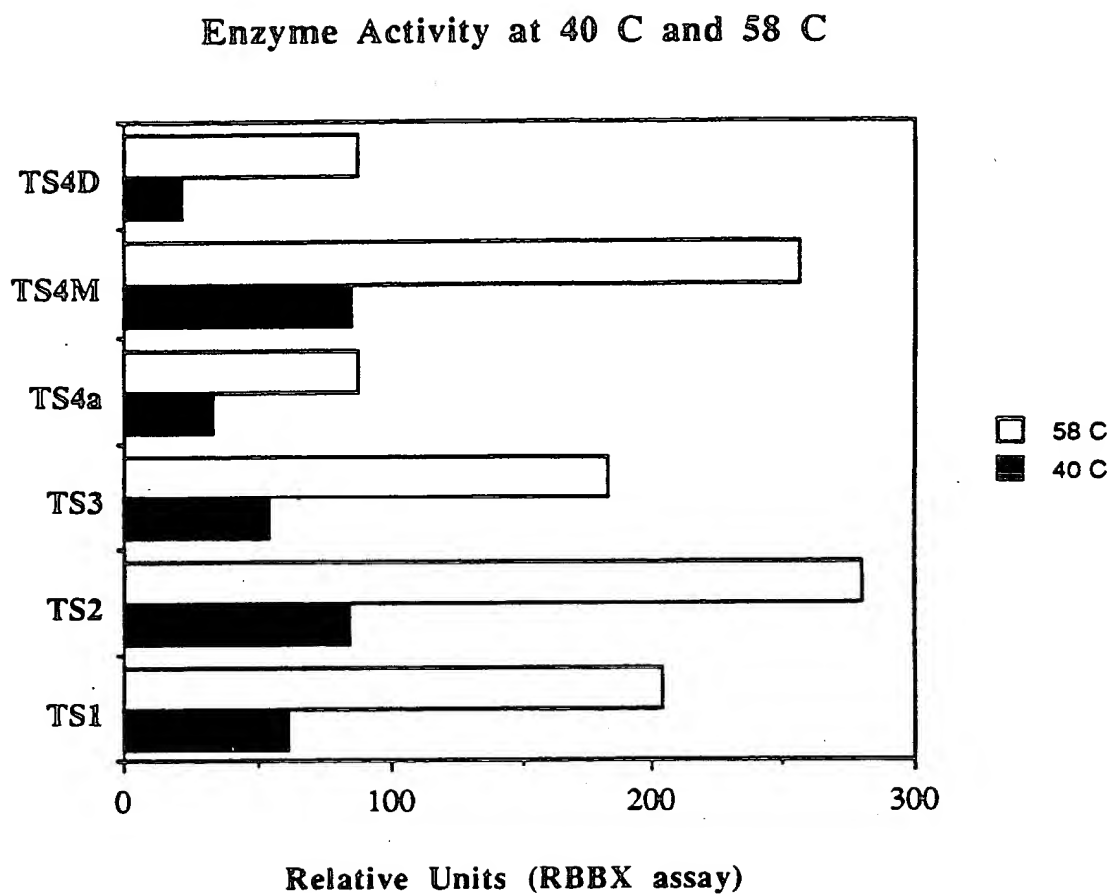
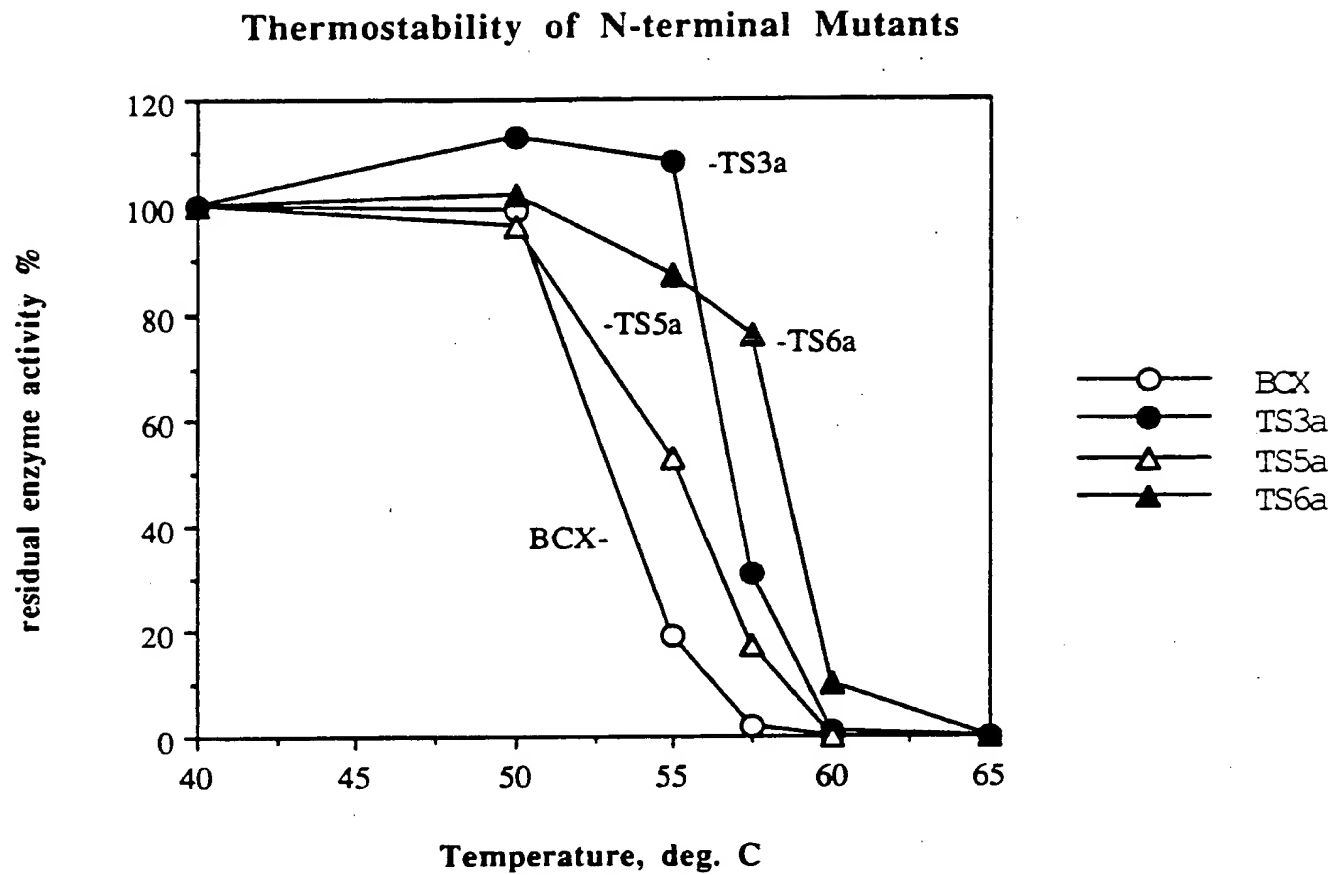


FIGURE 15

**FIGURE 16**

**FIGURE 17**

**FIGURE 18**

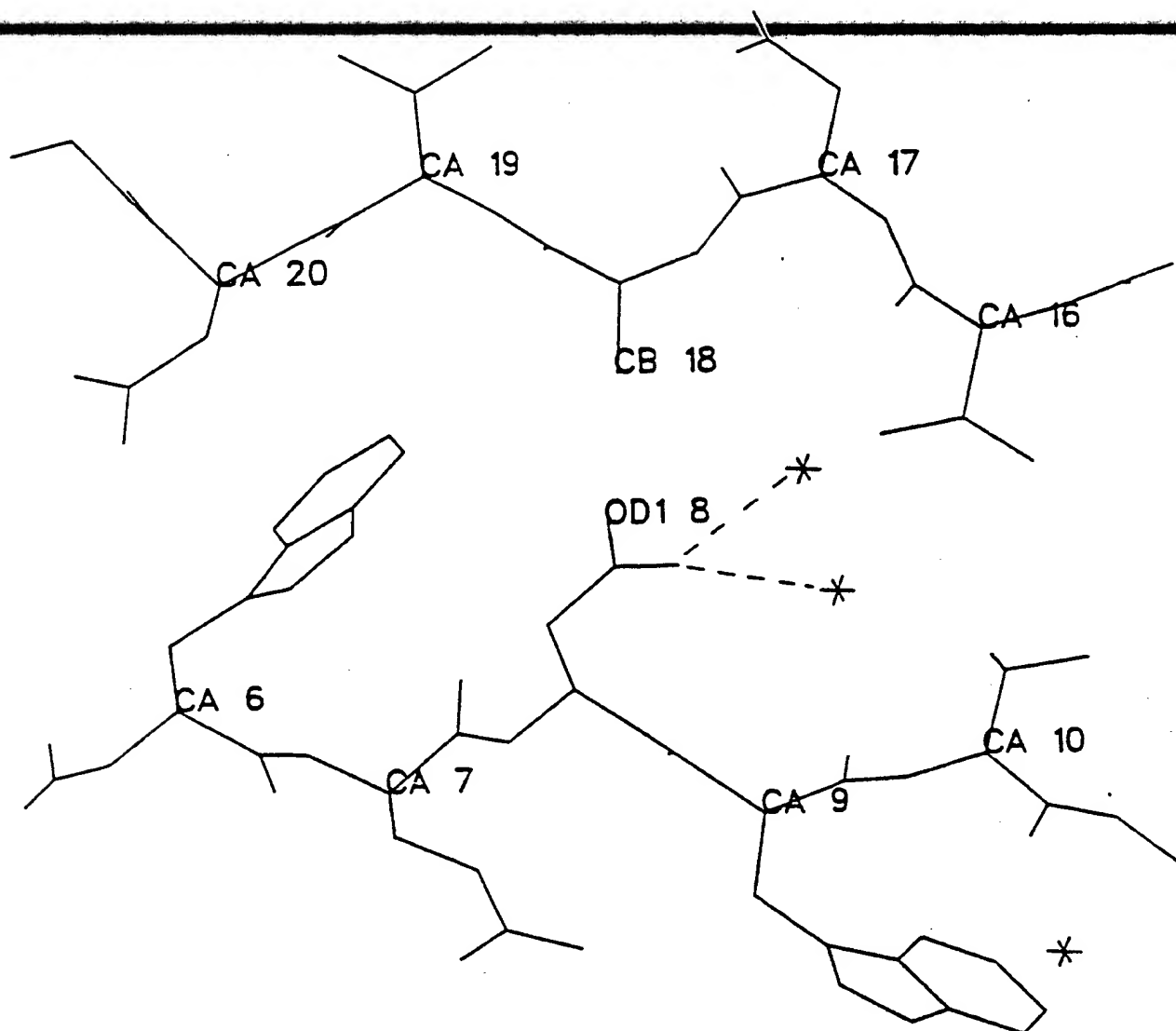
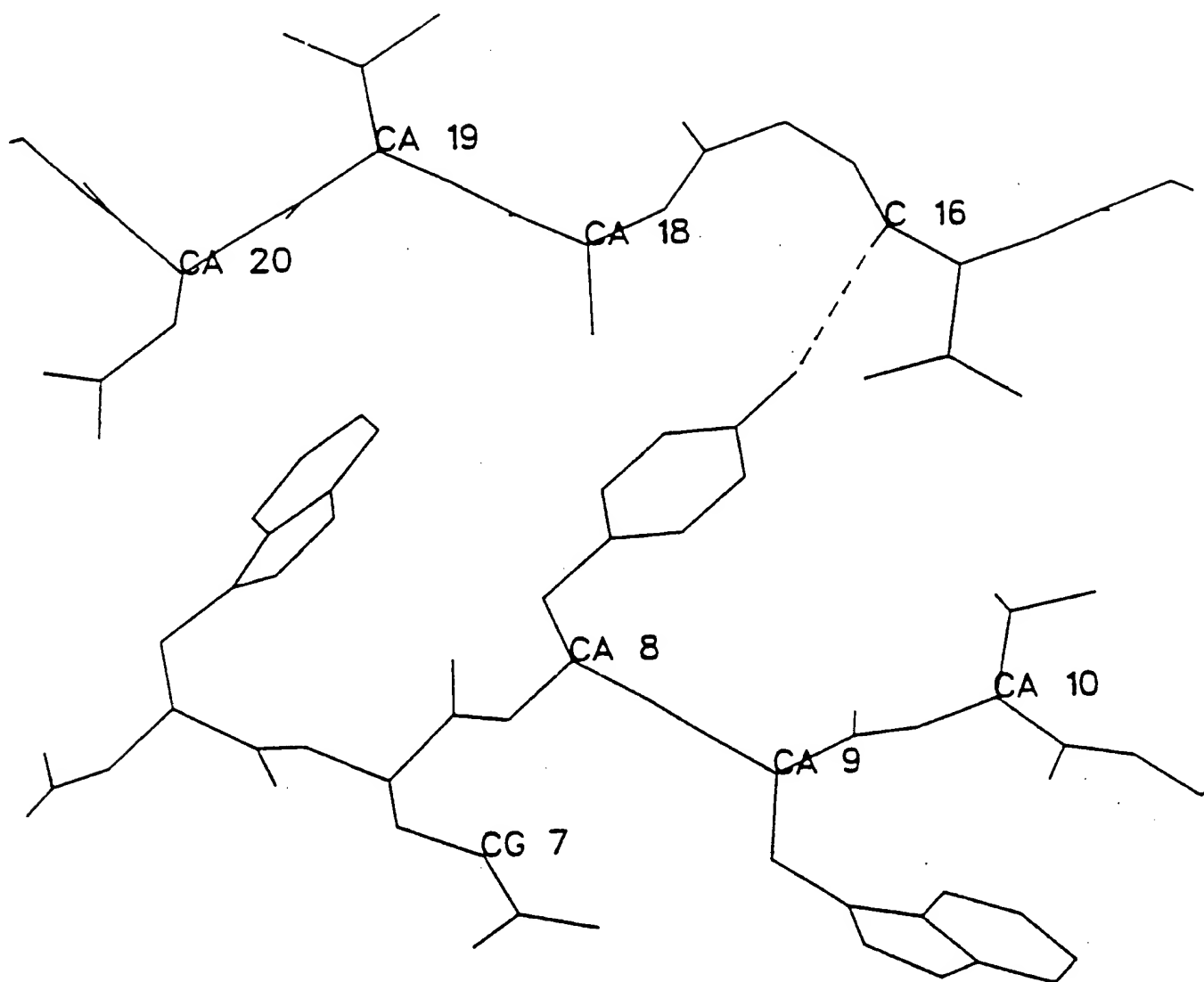


FIGURE 19

**FIGURE 20**

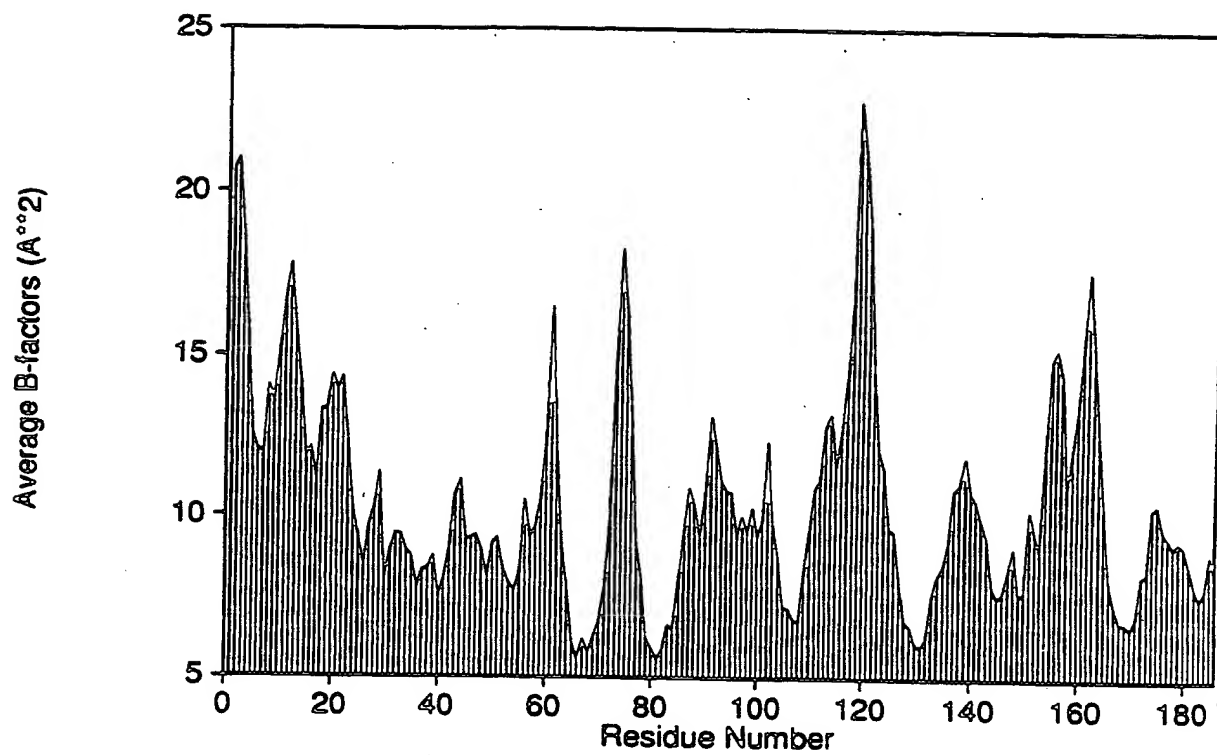


FIGURE 21

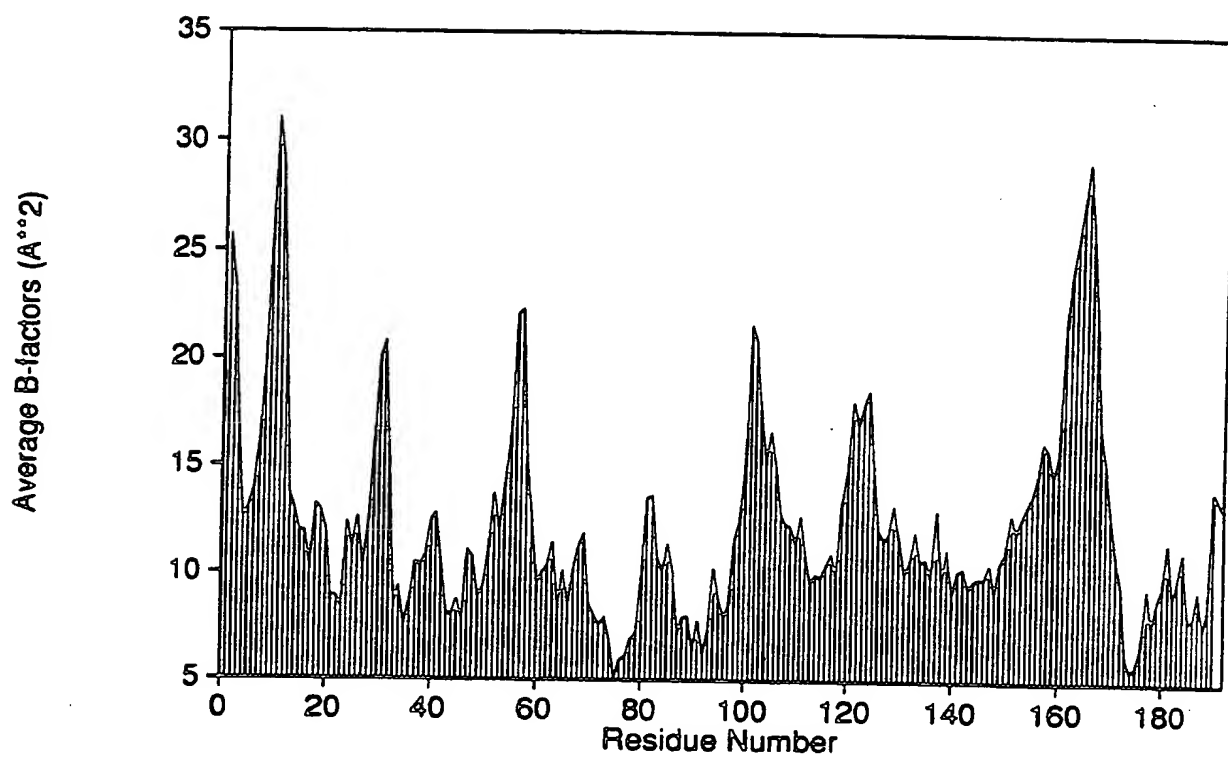


FIGURE 22

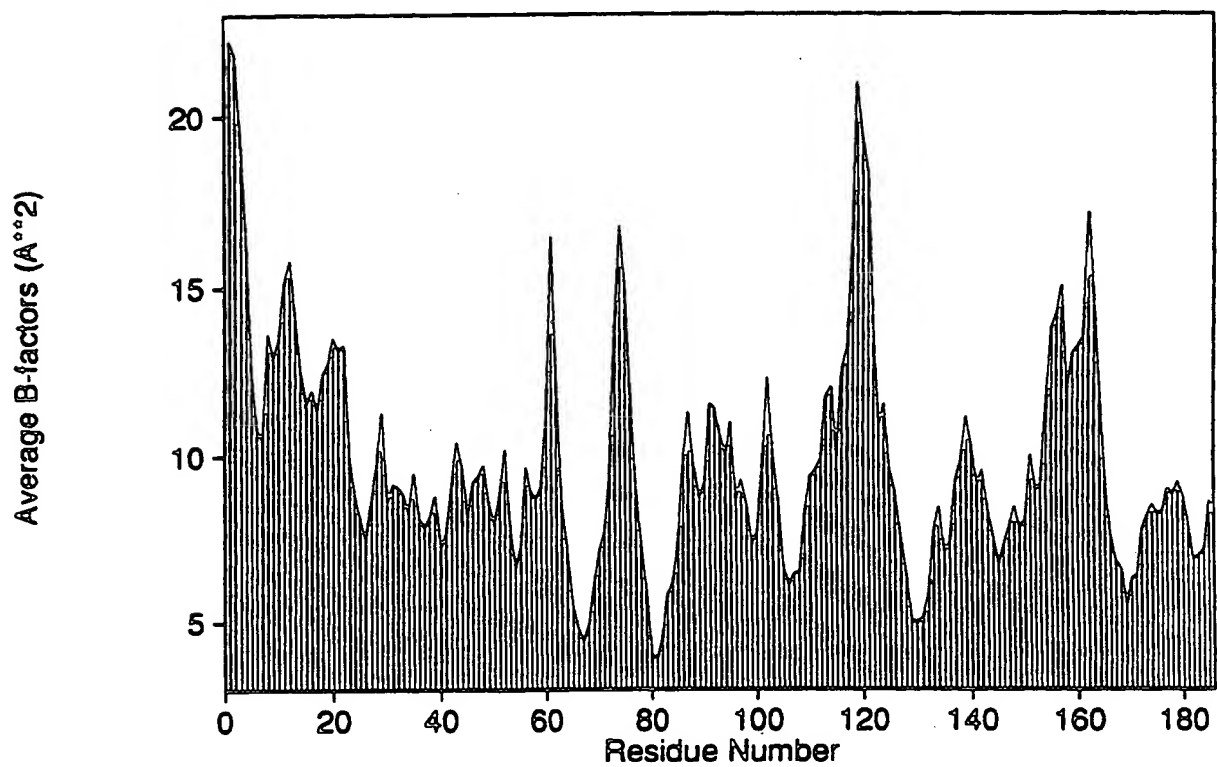


FIGURE 23

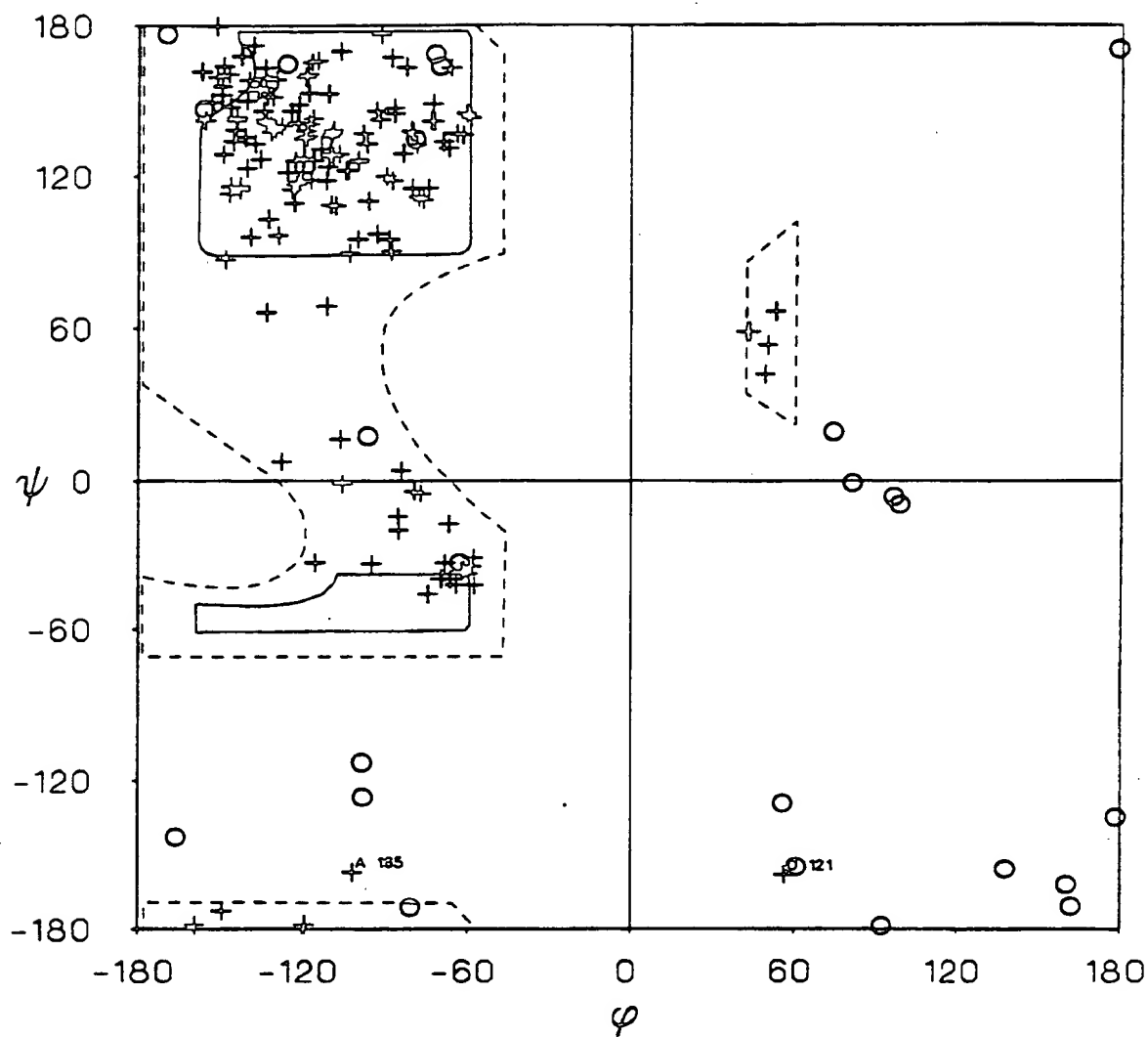


FIGURE 24

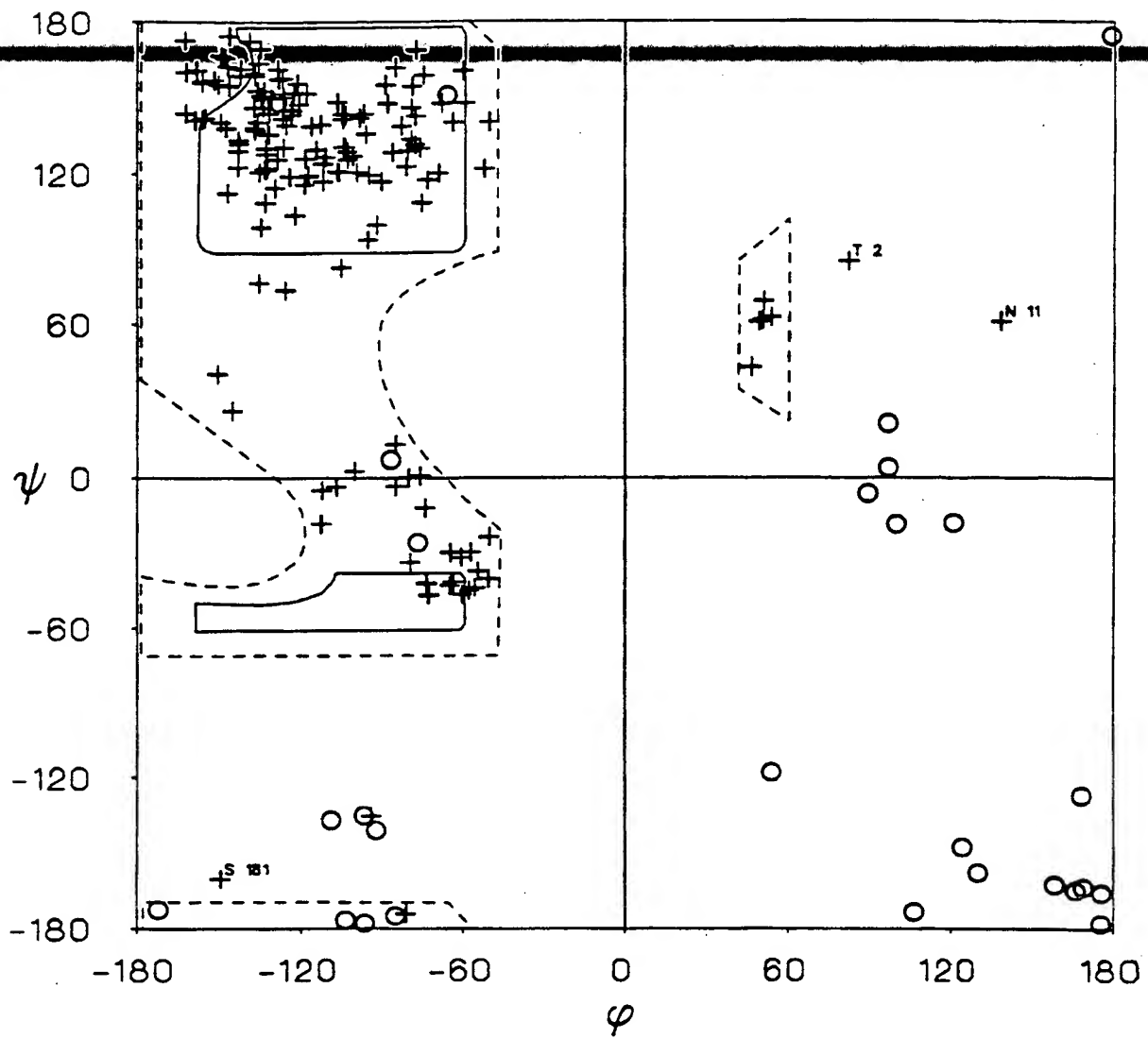


FIGURE 25

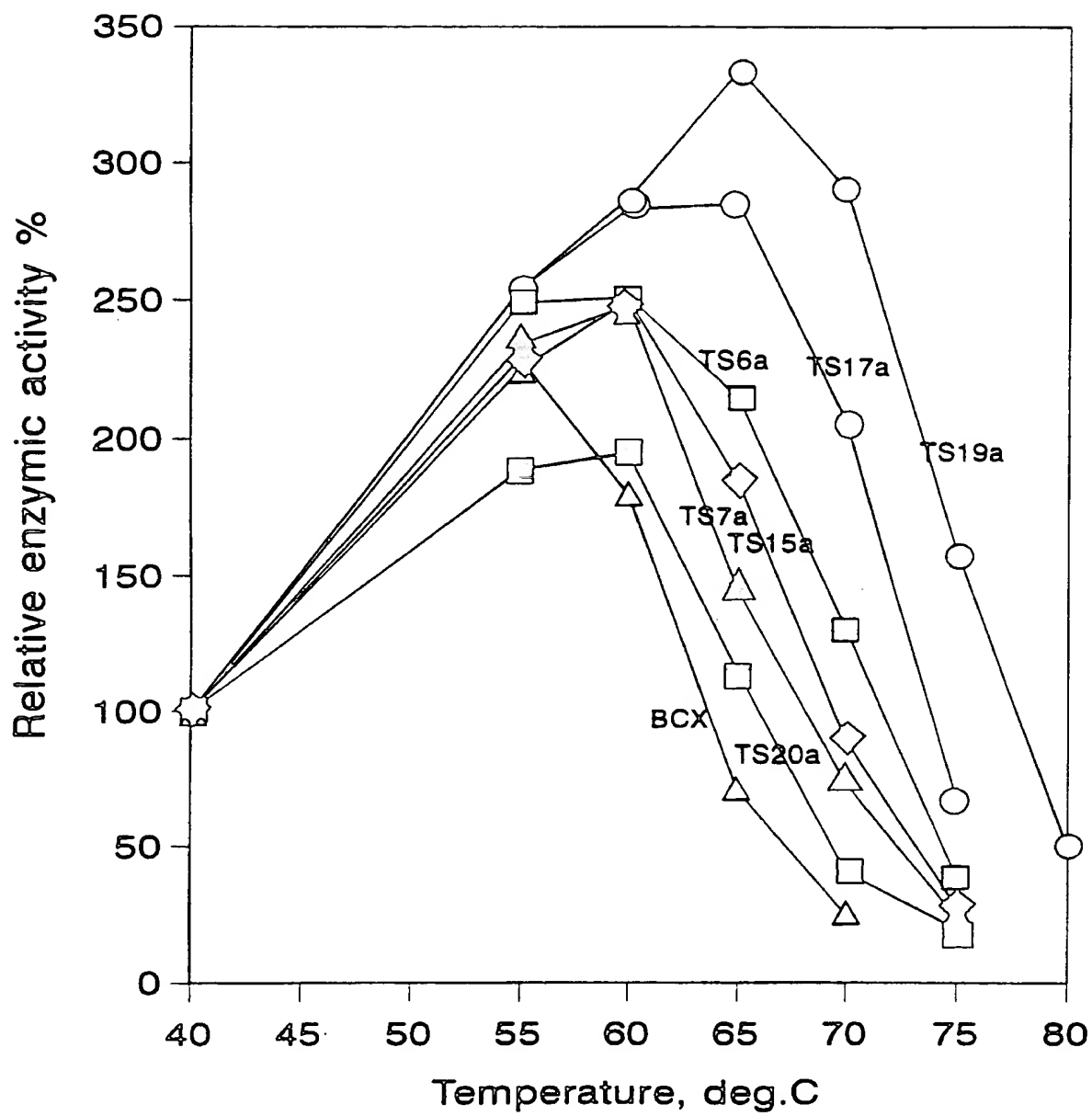


FIGURE 26

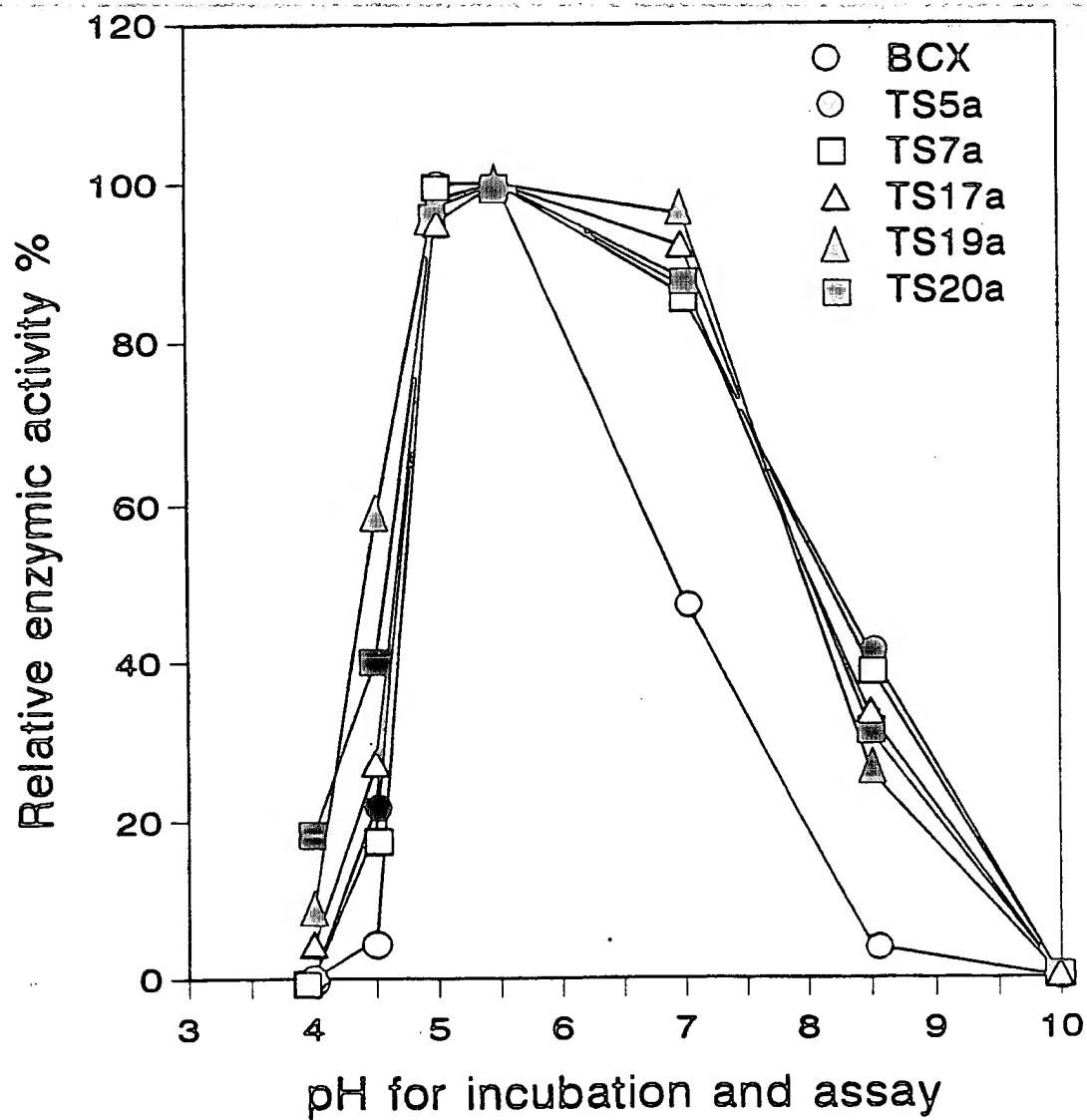


FIGURE 27

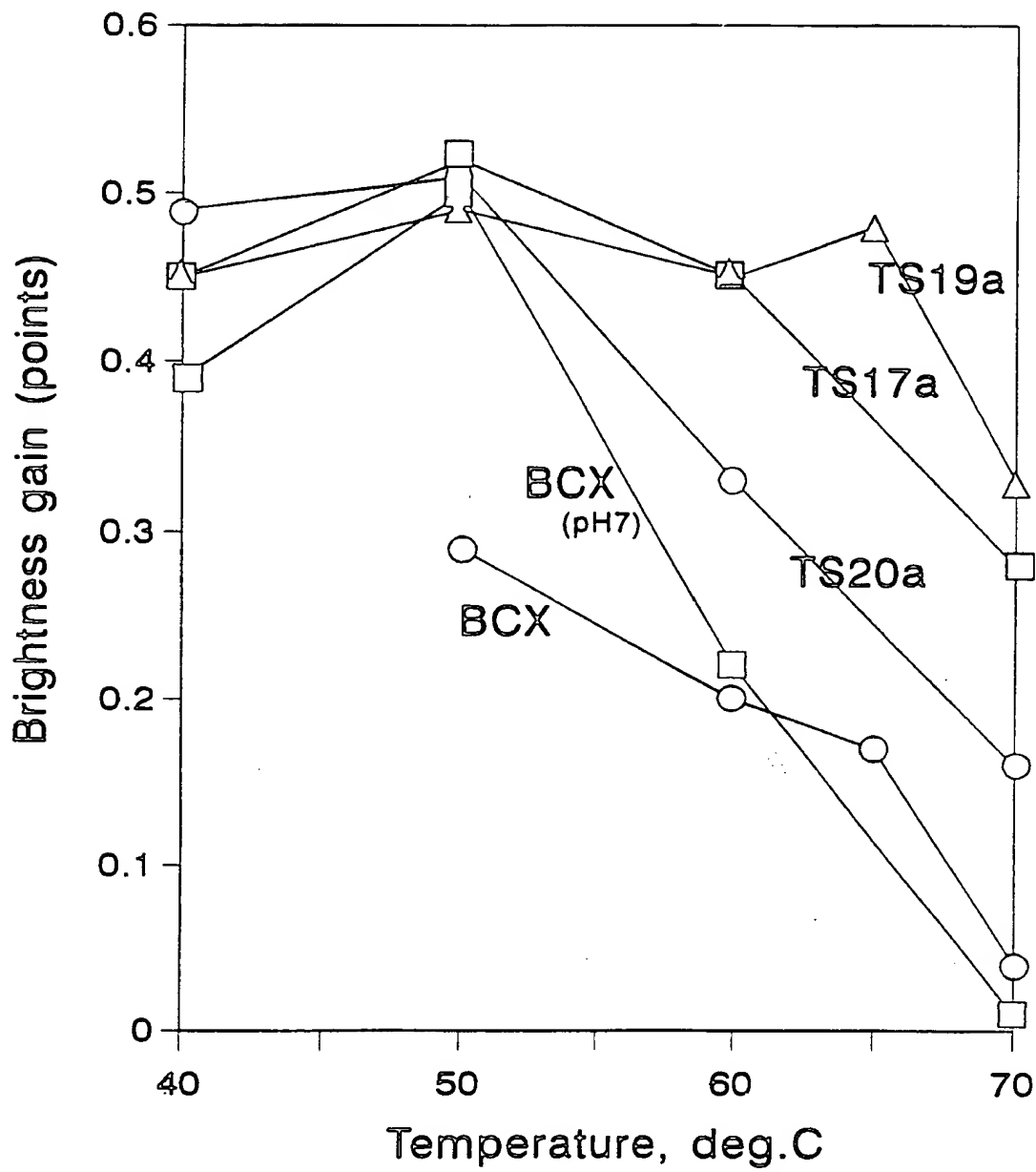


FIGURE 28

